201-15210

QUAT HPV CHALLENGE TASK GROUP
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April 27, 2004

Administrator Michael O. Leavitt
US Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116
Attention: Chemical Right-to-Know Program
Via E-mail: oppt.ncic@epa.gov and chem.rtk@epa.gov

Re: Submission of Test Plan and Robust Summaries for Quats

Dear Administrator Leavitt:

The Quat HPV Challenge Task Group is pleased to submit the attached test plan and robust summaries for the following chemicals for the US HPV Challenge Program, AR-201:

Chemical Name	CAS RN
Dimethylaminoethylacryalte methylchloride	44992-01-0
Dimethylaminoethylacryalte dimethylsulfate	13106-44-0
Dimethylaminoethylmethacryalte methylchloride	5039-78-1
Dimethylaminoethylmethacryalte dimethylsulfate	6891-44-7

You will note that the Quat HPV Challenge Task Group originally committed to sponsor two compounds under the US HPV Challenge Program: CAS RN 44992-01-0 and 5039-78-1. We are expanding this submission to include CAS RN 13106-44-0 and 6891-44-7 due to their similar toxicity and physical chemical properties.

Please do not hesitate to contact me at 202-419-1500 or bobf@regnet.com if I can provide any further clarification.

Sincerely,

Robert J. Fensterheim
Executive Director

201-15210B1

Test Plan for Quats

Dimethylaminoethylacrylate methylchloride [CAS No. 44992-01-0]

Dimethylaminoethylacrylate dimethylsulfate [CAS No. 13106-44-0]

Dimethylaminoethylmethacrylate methylchloride [CAS No. 5039-78-1]

Dimethylaminoethylmethacrylate dimethylsulfate [CAS No. 6891-44-7]

QUAT HPV CHALLENGE TASK GROUP

c/o RegNet Environmental Services

1250 Connecticut Avenue, N.W., Suite 700

Washington, D.C. 20036

Members of the Consortium:

Ciba Specialty Chemicals Corporation

Atofina Chemicals, Inc. (formerly Elf Atochem NA, Inc.)

Röhm GmbH

SNF Inc.

Summary

The member companies of the Quat HPV Challenge Task Force hereby submit for review and public comment their test plan for the family of chemical substances known as "quats" under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Challenge Program.

The quaternary ammonium salts of the esters of acrylic and methacrylic acid, dimethylaminoethylacrylate and dimethylaminoethylacrylate represent a category for the purposes of the HPV Challenge Program. Briefly, the ester precursor is produced by reaction of dimethylaminoethanol with acrylic acid or methacrylic acid, producing either dimethylaminoethylacrylate (ADAM) or dimethylaminoethylmethacrylate (MADAM), respectively. These esters differ from each other by one carbon in the acrylic chain. The tertiary amine moiety is caustic and lacks stability. In order to alleviate these characteristics, the tertiary amine is reacted with either methyl chloride (MC) or dimethyl sulfate (DMS) to produce a more stable and less caustic quaternary amine salt. So, both ADAM and MADAM have both a methyl chloride salt (ADAMMC and MADAMMC) and a dimethyl sulfate salt (ADAMDMS and MADAMDMS). The toxicity and physical chemical properties of these quaternary ammonium salts are very similar, as would be expected. The tertiary amine salts have been used as the surrogate for the category as they have been tested extensively (SIDS Dossier ID 2439-35-2 [ADAM] and SIDS Dossier ID 2867-47-2 [MADAM]).

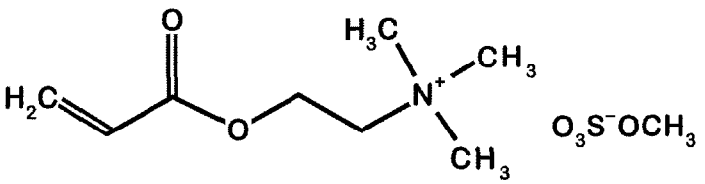
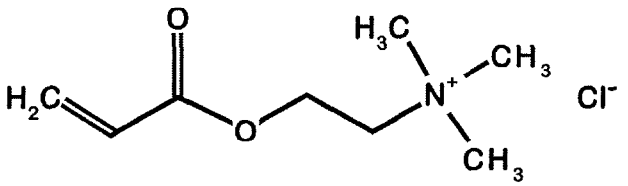
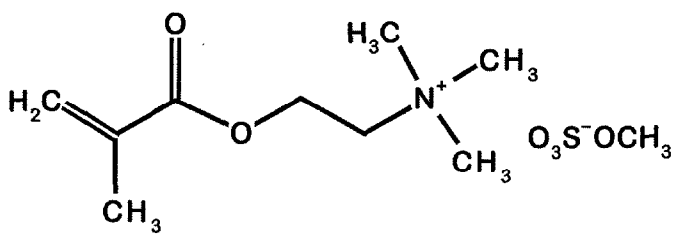
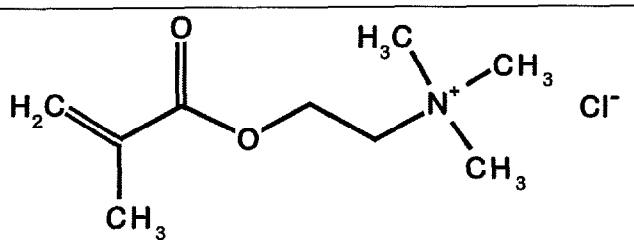
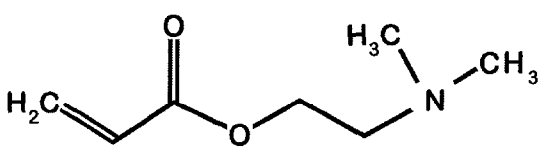
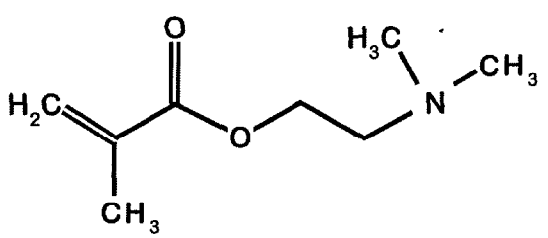
Note: Since the initiation of the HPV program, the production volume of ADAMDMS and both MADAM salts have dropped substantially. It is unlikely that the current magnitude of production still qualifies these substances as HPV chemicals.

Proposed Test Plan

No further testing is necessary on this category.

Identity, Chemistry and Basis of Category

The quaternary ammonium salts of the acrylic acid esters dimethylaminoethylacrylate and dimethylaminoethylmethacrylate represent a category for the purposes of the HPV Challenge Program. Briefly, the ester precursor is produced by reaction of dimethylaminoethanol with acrylic acid or methacrylic acid, producing either dimethylaminoethylacrylate (ADAM, CASRN 2439-25-2) or dimethylaminoethyl-methacrylate (MADAM, CASRN 2867-47-2). These esters differ from each other by a methyl group on the acrylic chain. The tertiary amine moiety is caustic and lacks stability. In order to alleviate these characteristics, the tertiary amine is reacted with either methyl chloride or dimethyl sulfate to produce a more stable and less caustic quaternary amine salt. So, both ADAM and MADAM have both a methyl chloride (MC) salt (ADAMMC and MADAMMC) and a dimethyl sulfate (DMS) salt (ADAMDMS and MADAMDMS). The toxicity and physical chemical properties of these quaternary ammonium salts are very similar, as would be expected. The tertiary amine salts have been used as surrogates for the category as they has been tested extensively with IUCLID and SIDS documents available on both: (SIDS Dossier ID 2439-35-2; SIDS Dossier ID 2867-47-2). The structures of the quaternary ammonium salts as well as their acid ester precursors are shown below.

Quaternary Ammonium Salts	
	Dimethylaminoethylacrylate, dimethyl sulfate (ADAMDMS, CASRN 13160-44-0)
	Dimethylaminoethylacrylate, methyl chloride (ADAMMC, CASRN 44992-01-0)
	Dimethylaminoethylmethacrylate, dimethyl sulfate (MADAMDMS, CASRN 6891-44-7)
	Dimethylaminoethylmethacrylate, methyl chloride (MADAMDMS, CASRN 5039-78-1)
Esters of Acrylic and Methacrylic Acids	
	Dimethylaminoethylacrylate (ADAM, CASRN 2439-35-2)
	Dimethylaminoethylmethacrylate (MADAM, CASRN 2867-47-2)

Summary of Exposure and Test Data

ADAM and MADAM are quaternized with either methyl chloride or dimethyl sulfate in a closed system to produce ADAMMC, ADAMDMS, MADAMMC and MADAMDMS. These quaternary ammonium salts are then polymerized to form homopolymers and copolymers with other monomers (mainly with acrylamide), in a closed system to produce cationic water-soluble polymers. Polymerization is the only use of these chemicals. The polymers are used for waste-water and sludge treatment, paper manufacture, mining and other uses. There is virtually no human exposure to the quaternized salts.

The quaternary salts have very low environmental toxicity. They have very low toxicity to fish and daphnia and have an algal LC50 greater than 1 mg/L. They have a low order of toxicity to laboratory animals. They are not irritating to the skin, moderately irritating to eyes and are dermal sensitizers

ADAM has been tested in subchronic gavage studies and induces gastric hyperplasia in the stomach. It is not teratogenic and docs it does not induce reproductive effects (SIDS Dossier ID 2439-35-2).

We conclude that there is sufficient data on the quats and their unquaternized acrylic acid esters that no further testing is needed on this category at this time.

Test Data

The test conducted on the quats as well as on the esters of acrylic and methacrylic acid are shown in the following table:

Environmental Studies	ADAM MC	ADAM DMS	ADAM	MADAM MC	MADAM DMS	MADAM
Acute fish toxicity	✘	✘	✘	✘	✘	✘
Acute daphnid toxicity	✘	✘	✘	✘	✘	✘
Acute algal inhibition	✘	✘	✘	✘	✘	✘
Chronic algal inhibition	✘	✘	✘	✘	✘	✘
Effect on bacteria	✘	✘	✘	✘	✘	✘
Biodegradability	✘	✘	✘	✘	✘	✘
Human Health Studies						
Acute oral toxicity	✘	✘	✘	✘	✘	✘
Ames test	✘	✘	✘	✘	✘	✘
Primary skin irritation	✘	✘	✘	✘	✘	✘
Acute eye irritation	✘	✘	✘	✘	✘	✘
Sensitization	✘	✘	✘	✘	✘	✘
Human lymphocytes	✘	✘	✘	✘	✘	✘
Mouse lymphoma	✘	✘	✘	✘	✘	✘*
Subchronic toxicity	✘	✘	✘	✘	✘	✘
Reproductive effects	✘	✘	✘	✘	✘	✘

* Chinese hamster cells were tested rather than mouse lymphoma

TOXICITY TO AQUATIC ORGANISMS

Tests Conducted on Aquatic Organisms: ADAMMC			
Study	**Species**	**Strain**	**Result**
Acute Toxicity (96h)	Fish	Zebra Fish	LC50 > 100 mg/l
Immobilization (48h)	Daphnia	*Dapnia magna*	EC50 > 100 mg/l
Growth inhibition (72h)	Algae	*Scenedesmus subspicatus*	1 < IC50 < 10 mg/l
Growth inhibition (72h)	Algae	*Scenedesmus subspicatus*	IC50 = 0.65 mg/l
Tests Conducted on Aquatic Organisms: ADAMDMS			
Acute Toxicity (96h)	Fish	Zebra Fish	LC50 > 100 mg/l
Immobilization (48h)	Daphnia	*Dapnia magna*	EC50 > 100 mg/l
Growth inhibition (72h)	Algae	*Scenedesmus subspicatus*	1 < IC50 < 10 mg/l
Tests Conducted on Aquatic Organisms: MADAMMC			
Acute Toxicity (96h)	Fish	Zebra Fish	LC50 > 100 mg/l
Immobilization (48h)	Daphnia	*Dapnia magna*	EC50 > 100 mg/l
Growth inhibition (72h)	Algae	*Scenedesmus subspicatus*	IC50 > 100 mg/l
Tests Conducted on Aquatic Organisms: MADAMDMS			
Acute Toxicity (96h)	Fish	Zebra Fish	LC50 > 100 mg/l
Immobilization (48h)	Daphnia	*Dapnia magna*	EC50 > 100 mg/l
Growth inhibition (72h)	Algae	*Scenedesmus subspicatus*	10 < IC50 < 100 mg/l
Tests Conducted on Aquatic Organisms: ADAM (*i.e.*, non-quaternized)*			
Acute Toxicity (96h)	Fish	Zebra Fish	LC50 > 8.5 mg/l
Immobilization (48h)	Daphnia	*Dapnia magna*	EC50 > 9.9 mg/l
Growth inhibition (72h)	Blue-green	*Scenedesmus subspicatus*	IC_A50 = 0.23 mg/l
Tests Conducted on Aquatic Organisms: MADAM (*i.e.*, non-quaternized)*			
Acute Toxicity (96h)	Fish	Goldfish	LC50 = 139.5 mg/l
Immobilization (48h)	Daphnia	*Dapnia magna*	EC50 = 53mg/l

*Data from OECD HPV SIDS dossier

Quaternized ammonium salts have a low order of aquatic toxicity. The table above summarizes the aquatic toxicity tests carried out. These monomers have no toxicity to multi-cellular organisms. For fish, the LC50s at 96 hours are all greater than 100 mg/L (Calmels, 1994a; Calmels, 1994b; Calmels, 1994c). Similarly, for daphnia, the EC50s (immobilization) at 48 hours are all greater than 100 mg/L (Calmels, 1994d; Calmels, 1994e; Calmels, 1994f). They demonstrate significant effects on the growth of the most sensitive algal test species *Scendesmus subspicatus*, especially the ADAM quats (Licata-Messana, 1994a; Licata-Messana, 1994b). This is common among quaternized ammonium salts. However, in this case, the effect is most likely the result of the hydrolysis of the residual ester of acrylic acid to acrylic acid (ADAM) and methacrylic acid (MADAM). Acrylic acid demonstrates a high degree of inhibition on the growth of this species (EC50/72 hours = 0.004 mg/l) while methacrylic acid demonstrates a lower effect (1 < IC50 < 10 mg/l). The aquatic toxicity of ADAM and MADAM from their respective OECD HPV SIDS dossiers has been included for completeness (SIDS Dossier ID 2439-35-2).

ENVIRONMENTAL FATE

Environmental Fate Studies		
Substance	**Study**	**Result**
ADAMMC	OECD TG 302B: Inherent Biodegradability, Zahn-Wellens Test	85% in 27 days
MADAMMC	OECD TG 301B: Ready Biodegradability. CO_2 Evolution (Modified Sturm Test)	69% in 28 days

ADAMMC has been tested for inherent biodegradability (Wehrhahn, 1999). It was found to be biodegradable to 85% in 27 days. MADAMMC has been tested for ready biodegradability (Thiébaud, 1996) and was found to be biodegradable to 69% in 28 days. From these test results it can be deduced that all the quats are highly biodegradable.

No further environmental testing is necessary for this category of chemicals.

ACUTE TOXICITY

Acute Toxicity Tests Conducted *In Vivo* on ADAMMC			
Study	**Species**	**Strain**	**Result**
Acute Oral Toxicity	Rat	Sprague-Dawley	LD50 = 1600 mg/kg
Primary Skin Irritation	Rabbit	New Zealand White	0.0 (Not irritating to skin)
Acute Eye Irritation	Rabbit	New Zealand White	25 on Day 1 (Moderate)
Sensitization	Guinea Pig	Dunkin-Hartley	Sensitizing
Acute Toxicity Tests Conducted *In Vivo* on MADAMMC			
Study	**Species**	**Strain**	**Result**
Acute Oral Toxicity	Rat	Sprague-Dawley	LD50 = 1300 mg/kg
Acute Toxicity Tests Conducted *In Vivo* on ADAM*			
Study	**Species**	**Strain**	**Result**
Acute Oral Toxicity	Rat	Sprague-Dawley	LD50 = 455 mg/kg
Acute Dermal Toxicity	Rat	Sprague-Dawley	LD50 = 419 mg/kg
Acute Inhalation Toxicity	Rat	Sprague-Dawley	LC50/4 hours = 0.066 mg/l
Primary Skin Irritation	Rabbit	New Zealand White	8.0 (Corrosive)
Acute Eye Irritation	Rabbit	New Zealand White	49 on Day 1 (Corrosive)
Sensitization	Guinea Pig	Hartley-Dunkin	Sensitizing
Acute Toxicity Tests Conducted *In Vivo* on MADAM*			
Study	**Species**	**Strain**	**Result**
Acute Oral Toxicity	Rat	Sprague-Dawley	LD50 = 1,550 mg/kg
Acute Dermal Toxicity	Rat	Sprague-Dawley	LD50 > 3,000 mg/kg
Acute Inhalation Toxicity	Rat	Sprague-Dawley	LC50/4 hours = 0.62 mg/l
Primary Skin Irritation	Rabbit	New Zealand White	5.97 (Corrosive)
Acute Eye Irritation	Rabbit	New Zealand White	Corrosive
Sensitization	Guinea Pig	Hartley-Dunkin	Sensitizing

*Data from OECD HPV SIDS dossier

Acute Toxicity

The acute oral toxicity of ADAMMC and MADAMMC are very similar. The results are summarized in the above table. The LD50s for both materials are around 1600 and 1300 mg/kg, respectively (Collier, 1985d; Clouzeau, 1990). ADAMMC is not irritating to the skin but produces moderate eye irritation (Collier, 1985b; Collier, 1985c). MADAMMC and ADAMMC are both dermal sensitizers (Collier, 1985a). In contrast, ADAM, which is a tertiary, not a quaternary amine, has an oral LD50 in the rat of 455 mg/kg due primarily to gastric toxicity (SIDS Dossier ID 2439-35-2). It causes eye and skin burns and is also a sensitizer.

No testing is necessary for the acute toxicity or irritancy of these materials.

Mutagenicity

Mutagenicity Tests on the Quaternized Acrylic Esters				
Test Substance	**Ames Salmonella Microsome**	**L5178 Mouse Lymphoma**	**Human Lymphocyte Cytogenetics**	**Mouse Micronucleus**
MADAMMC	Negative	Negative	Negative	Not Done
MADAMDMS	Negative	Negative	Negative	Not Done
ADAMMC	Negative	Negative	Negative	Not Done
Mutagenicity Tests on the Acrylic Esters**				
MADAM	Negative	Negative	Positive*	Negative
ADAM	Positive	Not Done	Positive	Negative

* Chinese hamster cells were tested

** Data from OECD HPV SIDS dossier (SIDS Dossier ID 2439-35-2; SIDS Dossier ID 2867-47-2).

ADAMMC, MADAMMC MADAMDMS have been tested *in vitro* for gene mutations (Adams, 1990b; Clouzeau, 1991a; Clouzeau, 1991b; Wollny, 1997) and chromosomal aberrations (Adams 1990a). They are negative in these mutagenicity studies. For

completeness, we have included the results from mutagenicity tests of ADAM and MADAM.

Repeated dose toxicity

Quaternized acrylate esters have not been tested in repeat dose toxicity studies. Rather, the tertiary amine acrylate ester, dimethylaminoethyl acrylate (ADAM) has been tested. Two oral administration studies have been located (SIDS Dossier ID 2439-35-2).

Study 1: Parental toxicity

One of the oral studies was conducted according to OECD Test Guideline 422 in compliance with GLP (SIDS Dossier ID 2439-35-2). This was a combined repeated dose toxicity study with the reproduction/developmental toxicity screening test. Groups of 12 Sprague Dawley (Crl: CD) rats were administrated doses of 0 (vehicle; corn oil), 4, 20, and 100 mg of ADAM per kg bodyweight per day by gavage. The dosing period for males was 43 days, and females were dosed from 14 days before mating to day 3 of lactation. The results were summarized below.

Males

At 100 mg/kg/day, the following adverse effects were observed; a transient suppression of body weight gain, a decrease in food consumption, thickening of the wall of the forestomach, pancreatico-duodenal lymph nodes. Hyperplasia of plasma cells in the pancreatico-duodenal lymph nodes was observed. Increase ratio in reticulocyte, platelet and segmented neutrophil counts and decrease in albumin was observed. At 20 and 100 mg/kg/day, ulceration, inflammatory cell infiltration and hyperplasia of the mucosa were observed in the forestomach. However, histopathological changes in forestomach were considered toxicologically insignificant because these changes were based on stimulative of this chemical. At 4 mg/kg/day, no effects were observed. The NOAEL for males was considered as 20 mg/kg/day.

Females

In 100 mg/kg/day group, 2 females out of 12 died. Thickening of the wall of the forestomach, pancreatico-duodenal lymph nodes and atrophy of the thymus were observed. Ulceration, inflammatory cell infiltration and hyperplasia of the mucosa in the

forestomach and hyperplasia of plasma cells in the pancreatico-duodenal lymph nodes were observed. At 4 and 20 mg/kg/day, no effects were observed. Thus the NOAEL for females was considered as 20 mg/kg/day.

The NOAEL for the repeat dose toxicity is considered to be 20 mg/kg/day for both sexes.

Reproductive Phase

Reproductive parameters such as mating index, fertility index, number of corpora lutea or implantations, implantation index, gestation index, delivery index, gestation length, parturition or maternal behavior were not effected by compound administration. There were no compound related changes in number of offspring, sex ratio, live birth index, and viability index or body weight. Additionally, no abnormal findings were observed at external features, clinical signs or necropsy. Therefore, there are no effects by the compound on the reproductive performance of the parent animals and growth of the offspring. The NOAELs for reproductive/development toxicity test are considered to be 100 mg/kg/day, the highest dose tested, for parental animals and offspring.

Study 2

The second study was conducted according to the OECD Test Guideline for repeated dose 90-day oral toxicity study in rodents [OECD TG 408] (SIDS Dossier ID 2439-35-2). Groups of Sprague Dawley (Crl: CD) rats were treated with doses of 0 (vehicle; peanut oil), 2, 10, and 50 mg/kg/day by gavage. The dosing period for males and females was 13 weeks. The results were summarized below.

Twenty rats/sex for control group, 10 rats/sex for low and intermediate dose-levels and 25 rats/sex for high dose-level were used. Thirteen males and 9 females died or were sacrificed moribund at 50 mg/kg/day. Twenty-one of these deaths (except one male) occurred during the exposure period. The cause of death was lung lesions, which were considered to be due to direct irritation from regurgitated stomach contents. No compound related clinical signs were observed at 2 and 10 mg/kg/day. Ptyalism and/or loud breathing were observed in a few animals at 50 mg/kg/day. Slight reduction in body weight gain was observed at 50 mg/kg/day in males and in all treatment groups in females. However, it was transient and not significant. There were no effects at 2 and 10 mg/kg/day. But, there was a slight increase in neutrophil counts and decrease in

lymphocyte counts. There were no changes in absolute and relative organ weight. There were no effects at food consumption, ophthalmology, blood biochemistry and urinalysis. In macroscopic examination, there were no effects at 2 and 10 mg/kg/day. At 50 mg/kg/day, grayish foci in the mucosa of the forestomach in 11/20 males and 13/19 females, enlargement of the pancreatic lymph nodes in 5/20 males and 6/19 females, dilatation or reddish color of the lungs in 7/20 males and 6/19 females were observed. In microscopic examination, hyperplasia/hyperkeratosis and edema and inflammatory cell infiltration of the forestomach submucosa were observed at 10 mg/kg/day. At 50 mg/kg/day, ulceration, hyperplasia/hyperkeratosis, infiltration or granulation tissue formation in the submucosa, oedema in mucosa and submucosa and necrosis of the mucosa/submucosa in forestomach, alveolar haemorrhage or edema and congestion in lungs were observed. These findings were considered to be a direct irritant effect or an effect of regurgitation of stomach contents.

The NOAEL for the repeat dose toxicity is considered to be 10 mg/kg/d

Reproductive phase

According to the OECD test guidelines 414, SD (Crl: CD) rats were administrated doses of 0 (vehicle; peanut oil), 10, 30 and 100 mg/kg/day by gavage. Females were dosed from day 6 to day 15 after mating was confirmed. The results are summarized below.

Twenty-five females for each group were used. Two females died at 30 mg/kg/day, one was killed prematurely at 100 mg/kg/day. Some clinical signs (principally loud breathing, piloerection, chromorhinorrhea, round back and dyspnea) were observed in a few female at the 30 and 100 mg/kg/day. No abortions occurred in any female. No total resorptions occurred in any female except one at 100 mg/kg/day. Reduction in food consumption and body weight gain were observed slightly at 100 mg/kg/day. In macroscopic examination, there were no effects at 10 mg/kg/day. At 30 and 100 mg/kg/day, gastrointestinal tract (gaseous dilatation or thickening of mucosa) were observed in 3/25 and 6/25 females, respectively. These findings were principally observed in the decedent animals. At 100 mg/kg/day, the post-implantation loss was slightly increased and the body weight of the fetuses was decreased. The number of live fetuses and sex-ratio were not affected.

In fetal observations: The following were found at 100 mg/kg/day. Twenty-seven/299 fetuses were malformed (14 fetuses from the same litter were dwarf, 13 other fetuses

from another litter suffered aphalangy). Two/144 fetuses were malformed (one fetus had a cleft palate, another fetuses presented hydrocephaly). Additionally, six dwarf fetuses suffered testicular ectopia. Reduced ossification or absence of ossification of many bones (head, vertebrae, sternebrae, limbs and paws) were also found at 30 mg/kg/day. The incidence for the absence of ossification of 6th sternebra was increase at 100 mg/kg/day. The NOAELs for development toxicity/teratogenicity test are considered to be 10 mg/kg/day for embryotoxicity and fetotoxicity, and to be 30 mg/kg/day for teratogenicity.

BACKGROUND INFORMATION

Method of manufacture

Quaternized ammonium salts (quats) are manufactured by derivitizing the corresponding tertiary amine. Methylchloride and dimethylsulfate are the derivitizing agents used. Production of the quaternary amine results in a more stable and cationic monomer.

Commercial Application

Quats are essentially copolymerized with acrylamide and sometimes with other monomers or homopolymerized to produce cationic, water-soluble polymers. These polymers are used for waste-water and sludge treatment, sugar processing, paper manufacture, mining and several other applications. The polymer contains trace levels of monomers.

Shipping

In United States, quats are generally polymerized at their manufacturing site. A percentage of quats enters interstate commerce, but generally only the polymer moves in commerce. When transported, it is sold in bulk as tank wagons or rail cars.

Worker Exposure

Quats are manufactured and polymerized in closed systems. They are easily pumped as they are liquid. No significant worker exposure occurs.

Consumer Exposure

There are no consumer applications for these chemicals.

Conclusion

This category of quaternized amino acrylate esters is used as starting monomers in closed systems. They are manufactured in zero discharge facilities with no significant human or environmental exposure. The tertiary amine, dimethylaminoethylacrylate, has been extensively tested. This substance has no reproductive or developmental toxicity and has

a NOAEL in rats of 10 mg/kg/day. Members of this category are more chemically stable, do not share the same propensity to cause gastric toxicity and therefore are expected to be substantially less toxic. In the absence of exposure and with substantial data on a structural congener, no further testing is recommended.

References

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201-15210B1

I U C L I D

Data Set

Existing Chemical	:	Substance ID: 44992-01-0
CAS No.	:	44992-01-0
TSCA Name	:	Ethanaminium, *N*,*N*,*N*-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, chloride
Structural formula	:	CH2=CHCOOC2H4N(CH3)3.Cl
Molecular formula	:	C8H16NO2.CL
Molecular weight	:	193.6729

Producer related part

Company	:	Quat HPV Challenge Task Group
Creation date	:	05.11.2003

Substance related part

Company	:	Quat HPV Challenge Task Group
Creation date	:	05.11.2003

Number of pages	:	35
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	Organic.
Physical status	:	Solid.
Purity	:	> 99%.
Remark	:	The commercial product is manufactured and shipped as a solution (75 – 80%) in water.

05.11.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Dimethylaminoethylacrylate, methyl chloride
05.11.2003

Choline chloride acrylate
05.11.2003

Dimethylaminoethyl acrylate methochloride
05.11.2003

[2-(acryloyloxy)ethyl]trimethylammonium chloride
05.11.2003

[(Acryyloxy)ethyl]trimethylammonium chloride
05.11.2003

ADAMMC
05.11.2003

DMAEA MC
05.11.2003

DMAEA MCQ
05.11.2003

1.3 IMPURITIES

Dimethylaminoethylacrylate (<0.1%).
05.11.2003

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

Sensitizing. Irritating to eyes.
05.11.2003

1.6.2 CLASSIFICATION

Not regulated.
05.11.2003

1.6.3 PACKAGING

1.7 USE PATTERN

Type	:	Industrial.
Category	:	Chemical industry; used in synthesis of water soluble polymers, flocculants, retention aids.
Remark	:	Commercial product is manufactured and shipped as a solution in water (75–80%).

05.11.2003

1.7.1 DETAILED USE PATTERN

Used in closed system to manufacture polymers. Polymers are water-soluble and cationic and are either copolymers with acrylamide and other monomers or homopolymers.
05.11.2003

1.7.2 METHODS OF MANUFACTURE

Manufactured by reaction of methyl chloride with dimethylaminoethylacrylate.
05.11.2003

1.8 REGULATORY MEASURES

None
05.11.2003

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

None.
05.11.2003

1.8.2 ACCEPTABLE RESIDUES LEVELS

Dimethylaminoethylacrylate (ADAM) at less than 0.1%.
05.11.2003

1.8.3 WATER POLLUTION

Not applicable.
05.11.2003

1.8.4 MAJOR ACCIDENT HAZARDS

Not applicable.
05.11.2003

1.8.5 AIR POLLUTION

Not applicable.
05.11.2003

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

Listed on all major chemical inventories (TSCA, EINECS, ECL, AICS, etc.).
05.11.2003

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

Not applicable.
05.11.2003

1.9.2 COMPONENTS

Pure substance (in aqueous solution).
05.11.2003

1.10 SOURCE OF EXPOSURE

None.
05.11.2003

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	=148.40°C.
Method	:	MPBPWIN v1.40.
Year	:	2003.
GLP	:	No.
Test substance	:	ADAMMC (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

07.11.2003

2.2 BOILING POINT

Value	:	=397.55°C
Method	:	MPBPWIN v1.40 (adapted Stein & Brown method).
Year	:	2003.
GLP	:	No.
Test substance	:	ADAMMC (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

07.11.2003

2.3 DENSITY

Type	:	Density.
Value	:	= 1.132 g/cm^3 at 20°C (80% solution in water).
Method	:	Other: no data
Year	:	No data.
GLP	:	No data.
Test substance	:	ADAMMC (80% solution in water).
Reliability	:	(4) not assignable. Only short information available (safety data sheet).

07.11.2003

2.3.1 GRANULOMETRY

Not applicable.
05.11.2003

2.4 VAPOUR PRESSURE

Value	:	=5.31 E-7 mm Hg at 25°C
Method	:	MPBPWIN v1.40 (modified Grain method).
Year	:	2003.
GLP	:	No.
Test substance	:	ADAMMC (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

07.11.2003

2.5 PARTITION COEFFICIENT

Partition coefficient	:	Octanol-water.
log Pow	:	= -3.10
Method	:	KOWWIN v1.66.
Year	:	2003
GLP	:	No.
Test substance	:	ADAMMC (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

07.11.2003

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water.
Value	:	1 E6 mg/l at 25°C.
Method	:	WSKOW v1.40.
GLP	:	No.
Test substance	:	ADAMMC (pure substance)
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions. Additionally, no melting point equation was used.

07.11.2003

Solubility in	:	Water.
Value	:	Completely miscible.
Method	:	Other: no data.
GLP	:	No data.
Test substance	:	ADAMMC (pure substance)
Reliability	:	(4) not assignable. Only short information available (safety data sheet).

07.11.2003

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	Does not flash.
Method	:	Other: no data.
Year	:	No data.
GLP	:	No data.
Test substance	:	MADAM MC (80% solution in water).
Reliability	:	(4) not assignable Only short information available (safety data sheet)

05.11.2003

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

Value	:	100 mPa.s
Method	:	Other: no data.
GLP	:	No data.
Test substance	:	ADAMMC (80%).
Reliability	:	(4) not assignable. Only short information available (safety data sheet).

05.11.2003

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	Air.
Method	:	AOPWIN v1.90.
Year	:	2003.
GLP	:	No.
Result	:	The atmospheric degradation behavior was assessed using AOPWIN (v. 1.90). An overall OH rate constant of 25.5215E-12 cm^3/molecule.sec was obtained. The following half-lives can be predicted under the chosen conditions: 0.419 days (12h-day, 1.5 E6 OH/cm^3); 5.029 hours. Overall ozone rate constant = 0.175 E-17 cm^3/molecule-sec. Half-life = 6.549 days (at 7 E11 mol/ cm^3)
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

07.11.2003

3.1.2 STABILITY IN WATER

Type	:	Abiotic (hydrolysis).
Method	:	HYDROWIN v1.67
Year	:	2003.
GLP	:	No.
Remark	:	The estimated hydrolysis half-life of this substance at: pH 7 = 9.001 years; ph 8 = 328.762 days
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

07.11.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	Volatility.
Media	:	Water – air.
Method	:	HENRYWIN v3.10.
Year	:	2003.
Remark	:	The value obtained for Henry's constant was calculated as: Bond contribution method: 6.96 E-15 atm-m^3/mole at 25°C (group contribution calculation incomplete). According to Thomas (1990), the substance may be considered as "not volatile from water". Henry's LC (VP/WSol estimate using EPI values) = 1.353 E-13 atm-m^3/mole

Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

07.11.2003

Type : Level III Fugacity Model
Media : Water – air – soil – sediment.
Method : BCFWIN v2.14.
Year : 2003.
Result : The value obtained from the Level III Fugacity Model are as follows:

	Mass Amount (%)	Half-Life (hr)	Emissions (kg/hr)
Air	2.49 E-7	9.45	1000
Water	45.3	360	1000
Soil	54.6	360	1000
Sediment	0.0755	1.44 E3	0

Persistence time = 421 hours.

Conclusion : Regardless of the media to which ADAMMC is released, virtually all at steady state is in the soil and water phases. Using the default emissions of equal amounts to soil, air, water and sediment (1000 kg/hr for each) the Level III model predicts that the distribution of ADAMMC will be 54.6% in soil, 45.3% in water, <0.1% in sediment, and virtually nothing in air.

Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

07.11.2003

3.3.2 DISTRIBUTION

Media : Air – biota – sediment(s) – soil – water.
Method : Calculation according to Mackay, Level 1.
Year : No data.
Remark : The following parameters were employed in this calculation:

Vapor pressure:	1.8 E-5 Pa	(20°C)	(calculated);
Molecular weight:	207.7 g/mol;		
water solubility:	ca. 6000 g/l	(20°C)	(calculated);
logPow:	–2.55	(25°C)	(calculated).

Result : The following environmental distribution was predicted:
water: ca. 100%; other environmental compartments below 0.001%.

Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

07.11.2003

3.4 MODE OF DEGRADATION IN ACTUAL USE

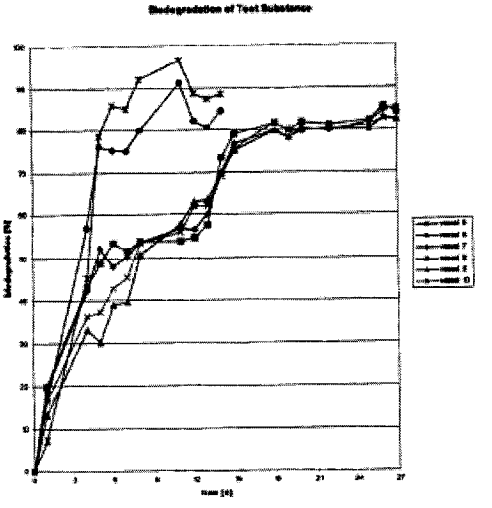
3.5 BIODEGRADATION

Type : Aerobic.
Reference Wehrhahn, D.
Inoculum : WWTP effluent.
Concentration : 60, 150 and 300 mg C/L.
Contact time : 27 days.
Degradation : = 85% after 27 days (average).

Result : Inherently biodegradable.
Deg. product : Not measured.
Method : OECD Guidelines for the Testing of Chemicals, No. 302 B (1981) "Inherent Biodegradability: Zahn-Wellens Test".
Year : 1999
GLP : Yes
Test substance : Adame-Quat (80% solution in water)
Method : A mixture containing the test substance, mineral nutrients and a fairly large amount of activated sludge in aqueous medium were agitated and aerated at room temperature for 27 days. Blank controls containing activated sludge and nutrient but no test material were run in parallel as well as a positive control (4-Ethoxybenzoic acid). Biodegradation was monitored in both by DOC (Dissolved Organic Carbon) determination in filtered samples. The ratio of eliminated DOC (corrected using the control), measured at each time interval to the initial DOC was expressed as the percentage biodegradation during the time interval. The DOC was measured 3 times a week with a DOC analyzer.
The results of this study showed that the carbon content of the test substance is biodegraded as follows:

Nominal Concentration (mg/l)	Percentage Biodegradation
60	86.5 at 14 days
150	84.8 at 14 days
300	82.7 at 27 days

The rate of biodegradation for each test concentration is graphically represented below:



Test substance : ADAMMC (80% solution in water).
Conclusion : ADAMMC was characterized as ultimately biodegradable.
Reliability : (1) valid without restrictions.
Guideline study.

07.11.2003

(1)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : Static.
Species : *Brachydanio rerio* (Zebra Fish)(Fish, fresh water).
Reference Calmels, R. (1994a).
Exposure period : 96 hours.
Unit : mg/l
LC0 : > 100
LC50 : Not observed.
LC50 : Not observed.
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 203, April 1984: "Fish, Acute Toxicity Test".
Year : 1994
GLP : No.
Test substance : ADAME MECL
Test procedure : Groups of 10 fresh water Zebra Fish (*Brachydanio rerio*) were exposed in a reconstituted medium at 23° C for 96 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Fish mortality was measured after 24, 48 and 96 hours.
Results : The results are given in the following table:

	Mortality		
Test Concentration (mg/L)	24 hours	48 hours	96 hours
0	0	0	0
1	0	0	0
10	0	0	0
100	0	0	0

Since the LC0 at 24, 48 and 96 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : ADAMMC (80% solution in water).
Conclusion : Under the conditions of this test, the test substance is not harmful to freshwater fish at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions.
Guideline study.

07.11.2003 (2)

Type : Static.
Species : *Danio rerio* (Zebra Fish)(Fish, fresh water).
Reference Wehrhan, D. (1999).
Exposure period : 96 hours.
Unit : mg/l
LC0 : 50
LC50 : 75
LC100 : 100
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 203, April 1984: "Fish, Acute Toxicity Test".
Year : 1994
GLP : Yes.

Test substance : Adame-Quat
Test procedure : The study was divided into a preliminary test over 48 hours and a main test over 96 hours. In the preliminary test the following nominal concentrations were used: 50, 100, 300, 700 and 1,000 mg/l. From 100 mg/l onward, mortalities were observed. Therefore, the main experiment was carried out with the following nominal concentrations: 50, 100, 150, 200, 250 and 300 mg/l. Nominal concentrations could not be verified because no specific analytical method was available. In the preliminary test, 5 fish were exposed to each concentration. in the main test, 10 fish were exposed to each concentration. The main test was carried out over 4 days. Mortalities and observable effects were recorded on a daily basis.
Results : The results are given in the following table:

	Mortalities			
Test Concentration (mg/L)	24 hours	48 hours	72 hours	96 hours
0	0	0	0	0
50	0	0	0	0
100	5	5	0	0
150	10	–	–	–
200	10	–	–	–
250	10	–	–	–
300	10	–	–	–

ADMMC was determined to have an LC50 at 96 hours of 75 mg/l, an LC100 of 100 mg/l and an LC0 of 50 mg/l.
Note: Slight deviations with respect to oxygen saturation occurred during the test (3% below required value).
Test substance : ADAMMC (80% solution in water).
Conclusion : Under the conditions of this test, the test substance has to be regarded as harmful (moderate concern) to *Danio rerio*.
Reliability : (1) valid without restrictions.
Guideline study.

07.11.2003 (3)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : Static.
Reference Calmels, R. (1994b).
Species : *Daphnia magna* (Crustacean, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
EC0 (immobilization) : > 100
EC50 (immobilization) : > 100 (Not observed).
EC100 (immobilization) : > 100 (Not observed).
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 202, Part 1, April 1984: "*Daphnia sp.*, Acute Immobilization Test".
Year : 1994
GLP : No.
Test substance : ADAME MECL
Test procedure : Groups of 10 fresh water daphnia (*Daphnia magna*) were exposed in a reconstituted medium at 23° C for 48 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test

substance were used. Immobilized daphnia were counted after 24 and 48 hours.

Results :

		Immobilization		
Concentration (mg/L)	No. of daphnia	No. after 24 hours	No. after 48 hours	% after 24 hours
0	20	0	1	5
1	20	0	1	5
10	20	0	0	0
100	20	0	0	0

Since the EC50 at 24 and 48 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : ADAMMC (80% solution in water)
Conclusion : Under the conditions of this test, the test substance is not harmful to *Daphnia magna* at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

07.11.2003 (4)

Type : Static.
Reference Wehrhahn, D. (1999b).
Species : *Daphnia magna* (Crustacean, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
EC0 (immobilization) : 40
EC50 (immobilization) : 120
EC100 (immobilization) : 320
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 202, Part 1, April 1984: "*Daphnia sp.*, Acute Immobilization Test".
Year : 1994
GLP : Yes.
Test substance : Adame-Quat
Test procedure : Groups of 25 new-born (age < 24 hours) *Daphnia magna* were exposed to nominal concentrations of 0, 5, 10,20, 40, 80, 160 and 320 mg/l. Nominal concentrations could not be verified because no specific analytical method was available. Each group, including the control, was divided into 5 parralel groups of 5 organisms. The test was carried out over 2 days. On day one and day two, immobilized daphnia were counted and recorded.

Results :

Conc. (mg/L)	No. of daphnia	Immobilization			
		After 24 hours		After 48 hours	
		Number	%	Number	%
0	25	0	0	1	4
5	25	0	0	1	4
10	25	0	0	1	4
20	25	0	0	2	8
40	25	0	0	1	4
80	25	0	0	9	36
160	25	4	16	11	60
320	25	25	100	–	100

ADMMC was determined to have an EC50 at 48 hours of 120 mg/l, an EC0 of 50 mg/l and an EC100 of 320 mg/l.

According to the EPA trimmed Spearman-Karber Method, the EC50s and their confidence limits are as follows

Point	Exposure Concentration	95% Confidence Limits	
		Lower	Upper
EC50 (24 hours)	202.52	182.95	224.19
EC50 (48 hours)	116.45	95.61	141.84

Test substance : ADAMMC (80% solution in water)
Conclusion : Under the conditions of this test, the test substance has to be regarded as slightly toxic to *Daphnia magna*. The test substance is of low toxic concern with respect to the species.
Reliability : (1) valid without restrictions
Guideline study.

07.11.2003 (5)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Type : Static.
Reference : Licata-Messana, L. (1994).
Species : *Scenedesmus subspicatus* (Algae, unicellular, fresh water).
Exposure period : 72 hours.
Unit : mg/l
EC_A50 (l) : Between 1 and 10 mg/l.
$EC_\mu50$ (l) : Between 10 and 100 mg/l.
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 201, June 1984: "Alga, Growth inhibition Test".
Year : 1994
GLP : No.
Test substance : ADAME MECL
Test procedure : Blue-green algae (*Scenedesmus subspicatus*) were exposed in a reconstituted medium for 72 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test

substance were used. Algal concentrations were measured after 24, 48 and 72 hours.

Results : The results are given in the following table:

GROWTH INHIBITION					
	Algal Concentration				
Concentration (mg/L)	Start	24 hours	48 hours	72 hours	% growth inhibition
0	10,000	188,340	2,248,344	13,850,004	0
1	10,000	380,004	1,923,336	12,283,332	11
10	10,000	230,004	806,676	2,933,340	79
100	10,000	180,000	306,672	300,012	98

GROWTH RATE INHIBITION		
Concentration (mg/L)	Growth rate	% growth rate inhibition
0	0.0612	–
1	0.0604	1
10	0.0384	37
100	0.0046	93

The EC(I)50 at 72 hours was determined to be:
Growth inhibition: $1 < EC_A50 < 10$
Growth rate inhibition: $10 < EC_\mu50 < 100$.

Test substance : ADAMMC (80% solution in water).
Conclusion : Under the conditions of this test, the test substance has to be considered as toxic to algae.
Reliability : (1) valid without restrictions.
Comparable to guideline study.

07.11.2003 (6)

Type : Static.
Reference Wehrhahn, D. (1999c).
Species : *Scenedesmus subspicatus* (Algae, unicellular, fresh water).
Exposure period : 96 hours.
Unit : mg/l
EC_A50 (I) : 1.1
$EC_\mu50$ (I) : 0.8
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 201, June 1984: "Alga, Growth inhibition Test".
Year : 1994
GLP : Yes.
Test substance : Adame-Quat
Test procedure : The test was carried out twice. In the first experiment the following concentrations were used: 0, 5, 10, 20, 40, 80, 160 and 320 mg/l. Nominal concentrations could not be verified since no specific analytical method was available. After 24 hours, no growth except in the control was observed, even in the lowest concentration. The test was stopped and carried out again with lower concentrations of the test substance and a control. each concentration and the control were prepared in quadruple. The nominal concentrations tested were 0.1, 0.2, 0.4, 0.8, 1.6, 3.2 and 6.4 mg/l. each

concentration and the controls were inoculated with approximately 10,000 algae per ml. The test was carried out over 96 hours. Once a day, the extinction of an aliquot of the test vessels was measured photometrically.

Results : The results are given in the following table:

Conc. (mg/L)	72 hours				96 hours			
	Area	Red (%)	Growth rate	Red (%)	Area	Red (%)	Growth rate	Red (%)
0	3.37	0	0.0541	0	8.27	0	0.0420	0
0.1	2.74	19	0.0496	8	7.03	15	0.0409	3
0.2	2.39	29	0.0590	-9	6.48	22	0.0480	-14
0.4	1.94	42	0.0573	-6	5.48	34	0.0488	-16
0.8	1.81	46	0.0604	-12	5.27	36	0.0510	-21
1.6	1.02	70	0.0513	5	3.12	62	0.0481	-15
3.2	0.53	84	0.0395	27	1.45	82	0.0409	3
6.4	0.19	94	0.0144	73	0.37	96	0.0237	44

The EC(I)50 at 72 hours was determined to be:
EC_A50 (growth)= 0.65
$EC_\mu50$ (growth rate) = 0.55

The EC(I)50 at 96 hours was determined to be:
EC_A50 (growth)= 1.1
$EC_\mu50$ (growth rate) = 0.8

Test substance : ADAMMC (80% solution in water).
Conclusion : Under the conditions of this test, the test substance has to be considered as toxic to algae.
Reliability : (1) valid without restrictions.
Comparable to guideline study.

07.11.2003 (7)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : Static
Reference Wehrhahn, D. (1999d)
Species : *Pseudomonas putida* (Bacteria).
Exposure period : 24 hours.
Unit : mg/l
EC50 : = 586
Analytical monitoring : No
Method : DIN 38 412 Teil 8 (Bringmann-Kühn, 1977)
Year : 1999
GLP : Yes
Test substance : Adame-Quat
Test procedure : The test was carried out at 30°C with the following nominal concentrations: 0, 3, 6, 12, 24, 49, 98, 195, 391, 781, 1563, 3,125, 3,250 and 12,500, 50,000, 100,000, 200,000 and 400,000 mg/l. Nominal concentrations could not be verified since no specific analytical method was available. Each concentration and the control were prepared in duplicate. each concentration was inoculated with 10 ml of a bacteria suspension with an extinction of 0.1 at λ = 436 nm. The bacteria were exposed to the test substance for 24 hours. Thereafter, an aliquot was taken from each test and

control vessel, which was diluted and aliquots from the resulting solutions were pipetted into Petri dishes filled with King B medium. Bacteria were distributed by means of a Drigalski spatula. The Petri dishes were incubated for one day at 30°C. The growth of the bacterial colonies on the Petri dishes was evaluated macroscopically.

Results : The results are given in the following table:

		Growth at dilution of 10^{-2}	
Concentration mg/l	**Dilution factor**	**Incubation A**	**Incubation B**
control	control	+++	+++
400,000	1:2	–	–
200,000	1:4	–	–
100,000	1:8	–	–
50,000	1:16	–	–
25,000	1:32	–	–
12,500	1:64	–	–
6,250	1:128	–	–
3,125	1:256	–	–
1,563	1:512	++	++
781	1:1024	++	++
391	1:2048	+++	+++
195	1:4096	+++	+++
98	1:8192	+++	+++
49	1:16392	+++	+++
24	1:32784	+++	+++
12	1:65568	+++	+++
6	1:131136	+++	+++
3	1:262772	+++	+++

The EC50 at 24 hours was determined to be 586 mg/l.

Test substance : ADAMMC (80% solution in water).
Conclusion : Under the conditions of this test, the test substance has to be regarded as slightly toxic to bacteria.
Reliability : (1) valid without restrictions.
Guideline study.

06.11.2003

(8)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Reference Clouzeau, J. (1990).
Units : mg/kg bw
Value : 1,600 < LD50 < 2,000.
Species : Rat.
Strain : Sprague-Dawley.
Sex : Male & female.
Number of animals : 5 male at all dose levels, and 5 female at 3 dose levels.
Body weight : Males: 188 ± 8 g; females: 144 ± 5 g.
Vehicle : Methylcellulose.
Doses : 500 – 2,900 mg/kg.
Observation : 15 days.
Method : OECD Guidelines for the Testing of Chemicals, Number 401, February, 1987: "Acute Oral Toxicity".
Year : 1990.
GLP : GLP.
Remark : LD50 calculated on the basis of pure active substance.
Test procedure : In a pilot study, the test substance was administered orally as is at a dose of 500 mg/kg body weight taking into account a specific gravity of d=1.12. Since the mortality in this study was 40%, a second test was conducted at doses of 500, 900, 1,600, 2,000 and 2,900 mg/kg for the males and 900, 1,600 and 2,000 mg/kg for the females. The test substance was administered in solution in 0.5% methylcellulose at a dose of 10 ml/kg. The animals were observed frequently during the immediate post-administration period and clinical signs were recorded.
Result : Animals showed sedation, ataxia, abdominal/side position and reduced food uptake. Dyspnia was observed in 1 male at the 1,600 mg/kg group and in most of the animals for a period of 1 hour in the 2,900 mg/kg group. 15 minutes following administration, a red-colored eye secretion was observed over 15 minutes in 2 males in the 1,600 mg/kg group, 2 males and 1 female in the 2,000 mg/kg group and 4 males in the 2,900 mg/kg group.
Cumulative mortality, in males, females and combined is given in the following table:

Sex	Dose mg/kg	Cumulative Mortality				Mortality %
		Day 1	Day 2	Day 5	Day 15	
Males	500	0	0	0	0	0
	900	0	0	0	0	0
	1,600	0	2	2	2	40
	2,000	5	5	5	5	100
	2,900	3	5	5	5	100
Females	900	0	1	1	1	20
	1,600	0	0	0	0	0
	2,000	5	5	5	5	100

The LD50 was determined to be between 1,600 and 2,000 mg/kg body

weight.

Test substance	:	ADAMMC (80% solution in water)
Conclusion	:	Under the conditions of this test, the LD50 of the test substance by the oral route in male rats is between 1,600 (40% mortality) and 2,000 mg/kg (100% mortality) body weight. The LD50 for females is slightly higher. The test substance is therefore regarded as being of low toxic concern.
Reliability	:	(1) valid without restrictions. Guideline study.

05.11.2003 (9)

Type	:	LD50
Reference		Collier, T. A. (1985a).
Units	:	mg/kg bw
Value	:	200 < LD50 < 2,000
Species	:	Rat.
Strain	:	Sprague-Dawley.
Sex	:	Male & female.
Number of animals	:	4 per dose (2 male and 2 female) in the rangefinding study and 10 per dose (5 male and 5 female) in the main study.
Body weight	:	Males: 101 – 111 g, females: 94 – 112g.
Vehicle	:	Water.
Doses	:	25 – 5,000 mg/kg bw.
Observation	:	14 days.
Method	:	OECD Guidelines for the Testing of Chemicals, Number 401, February, 1987: "Acute Oral Toxicity".
Year	:	1985
GLP	:	Yes
Remark	:	LD50 calculated on the basis of pure active substance.
Test procedure	:	A pilot study, was carried out at 4 pre-specified dose levels (25, 200, 2,000 and 5,000 mg/kg body weight) using groups of 4 rats (2 male and 2 female) in order to determine the highest of these level that produced no mortality. All rats were dosed once only by gavage using a metal canulla attached to a graduated syringe. The dose volume administered to each animal was calculated according to its body weight at the time of dosing. Animals were observed at 0.5, 1 and 4 hours following then once daily for 5 days, or until signs of toxicity were no longer apparent. Mortality and evidence of overt toxicity were recoded at each observation. A group of 10 rats (5 male and 5 female) were dosed once at 200 mg/kg body weight (the highest dose level in the pilot study that caused no mortality).

Result : An abnormal body carriage (hunched posture), lethargy, pilo-erection and decreased respiratory rate were observed in rats at 25, 200 and 2,000 mg/kg. In addition, body tremors, ataxia, increased salivation and dried blood around the eyes were seen at the 2,000 mg/kg dose level only. All animals dosed at 5,000 mg/kg died within 30 minutes of treatment.
Cumulative mortality, in males, females and combined is given in the following table:

		Cumulative Mortality				
Sex	Dose mg/kg	Day 1	Day 2	Day 5	Day 15	Mortality %
Males	25	0	0	0	0	0
	200	0	0	0	0	0
	2,000	0	1	1	1	50
	5,000	2	2	2	2	100
	Second Study					
	200	0	0	0	0	0
Females	0	0	0	0	0	0
	200	0	0	0	0	0
	2,000	0	0	0	0	0
	5,000	2	2	2	2	100
	Second Study					
	200	0	0	0	0	0

The LD50 was determined to be between 200 and 2,000 mg/kg body weight.

Test substance : ADAMMC (80% solution in water)
Conclusion : Under the conditions of this test, the LD50 of the test substance by the oral route in male rats is between 200 (0% mortality) and 2,000 mg/kg (100% mortality) body weight. The test substance is therefore regarded as being of low toxic concern.
Reliability : (1) valid without restrictions.
Guideline study.

05.11.2003 (10)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : Rabbit.
Reference Collier, T. A. (1985b).

Strain	:	New Zealand white.
Concentration	:	80 % active substance.
Exposure	:	Intact and abraded skin, occlusive.
Exposure time	:	4 hours.
Number of animals	:	3
Body weight	:	2.28 – 2.44 kg.
Observation	:	24, 48 and 72 hours.
Vehicle	:	None.
Result	:	Not irritating.
Method	:	OECD Guidelines for the Testing of Chemicals, Number 404, February, 1987: "Acute Dermal Irritation/Corrosion".
Year	:	1985
GLP	:	Yes.
Test procedure	:	Approximately 24 hours prior to the commencement of the test, each of a group of 3 rabbits by closely clipping the fur from the dorsal/flank areas. Only animals with a healthy epidermis were selected for the study. On the day of the test, a suitable test site was selected on the back of each rabbit. A quantity of 0.5 ml of the test material was introduced under a semi-occlusive patch which consisted of a 2.5 cm2 of surgical gauze 2 layers thick. The material was held in contact with the skin by the patch which was secured in position with 2 lengths of adhesive strapping. In addition, to prevent access to the patch, the trunk of each rabbit was wrapped in an elasticated corset. The material was kept in contact with the skin for a period of 4 hours. At the end of the exposure period, the corset was removed from each animal and the patches carefully taken off the test sites. Any residual material was immediately removed by gentle swabbing with cotton wool soaked in water. Patches were scored at 24, 48 and 72 hours according Draize (1959).
Result	:	According to the Draize evaluation scheme, a primary irritation index (intact/abraded skin) of 0.00 was determined. The following indices were obtained for the intact clipped skin:

	24 hours	48 hours	72 hours	Total
Erythema	0	0	0	0
Edema	0	0	0	0

The test substance was determined to be non-irritating to rabbit skin.

Test substance	:	ADAMMC (80% solution in water)
Conclusion	:	ADAME MC was determined to be non-irritating.
Reliability	:	(1) valid without restrictions. Guideline study.

07.11.2003 (11)

5.2.2 EYE IRRITATION

Species	:	Rabbit.
Reference		Collier, T. A. (1985c).
Strain	:	New Zealand white.
Concentration	:	80 % active substance.
Exposure	:	Eye.
Exposure time	:	Test substance was administered in a single application.
Number of animals	:	1

Body weight : 2.85 kg
Observation : 1 and 24 hours.
Vehicle : None.
Result : Moderately irritating.
Method : OECD Guidelines for the Testing of Chemicals, Number 405, February, 1987: "Acute Eye Irritation/Corrosion".
Year : 1985.
GLP : Yes.
Test procedure : A volume of 0.1 ml of the test material was instilled in the right eye of the rabbit by gently pulling the lower lid away from the eyeball to form a cup into which the test material was dropped. The upper and the lower eyelids were held together for about 1 second immediately after application to prevent loss of test material. Assessment of damage/irritation was made 1 hour and 24 hours following treatment according to the numerical scheme of Draize (1959). Examination of the eye was facilitated by use of a standard ophthalmoscope.
Result : A dulling of the normal luster of the cornea was observed at the 1-hour reading and by the 24-hour reading diffuse corneal opacity was observed. A diffuse beefy red coloration of the conjunctivae accompanied by severe swelling and extensive discharge was observed at the 1-hour reading. Similar reactions persisted at the 24-hour reading and were accompanied by areas of hemorrhage and necrosis over the conjunctivae and nictitating membranes. the results from the scoring according to the Draize method are given in the following table:

	1 hours	24 hours
Cornea		
E. Degree of Opacity	Dulling	1
F. Area of Opacity	4	1
Score (ExF) x 5	0	5
Iris (D)	1	1
Score (Dx5)	5	5
Conjuntivae		
A. Redness	3	3
B. Chemosis	4	4
C. Discharge	3	3
Score (A+B+C) x 2	20	20
Total Score	25	30

The test substance was determined to be moderately irritating to eyes.

Test substance : ADAMMC (80% solution in water)
Conclusion : ADAMMC was determined to be moderately irritating to eyes.
Reliability : (1) valid without restrictions.
Comparable to guideline study.

05.11.2003 (12)

5.3 SENSITIZATION

Species : Guinea pig.
Reference Collier, T.A. (1985d).
Concentration : Intradermal induction: 0.1% in water, intra-cutaneous.
Topical induction: 25% active substance, intra-cutaneous.
Challenge: undiluted, occlusive, epicutaneous.
Number of animals : 20
Method : OECD Guidelines for the Testing of Chemicals, Number 406 "Skin Sensitization" (Guinea Pig Maximization Test).
Year : 1985
GLP : Yes.
Test procedure : On Day 0, the experimental group was shaved. Into the shaved area were injected 0.1 ml of Freund's complete adjuvant, 0.1 ml of the test substance at 1% in water and 0.1 ml of a 50-50 mixture of 1% test material with Freund's adjuvant. On Day 7, the experimental group was shaved and test material at a concentration of 25% was applied to a 2 cm by 4 cm patch. Sleek water-proof adhesive strapping was used to hold patch in position. the dressing was removed after 48 hours. On Day 21, the experimental group was shaved and test material applied to the clipped, right flank of each animal. Vehicle alone was applied to the left flank. Both patches were covered with an overlapping length of aluminum foil and left for 24 hours. patches were removed and the exposure site washed and marked. On Day 24, the reaction sites were scored. Appropriate solvent controls were used in this study.
Result : No reaction was seen in the solvent controls. The results of the scoring out of a maximum of 4 are given in the following table:

Animal number	24 hours		48 hours	
	Test	Vehicle	Test	Vehicle
1	2	0	2	0
2	1	0	1	0
3	2	0	2	0
4	1	0	1	0
5	2	0	2	0
6	2	0	2	0
7	2	0	2	0
8	2	0	1	0
9	2	0	1	0
10	2	0	2	0
11	2	0	1	0
12	2	0	1	0
13	2	0	2	0
14	1	0	1	0
15	1	0	1	0
16	2	0	2	0
17	3	0	2	0
18	2	0	2	0
19	2	0	2	0
20	Died Day 7			

The test substance was determined to be a strong sensitizer.

Test substance : ADAMMC (80% solution in water)
Conclusion : ADAMMC was determined to be sensitizing.
Reliability : (1) valid without restrictions
Comparable to guideline study.

06.11.2003 (13)

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Reverse Mutation Assay (Ames Test).
Reference		Clouzeau J. (1991).
System of testing	:	*Salmonella typhimurium* TA1535, TA1537, TA1538, TA98 and TA100
Test concentration	:	10 – 5000 µg/plate
Metabolic activation	:	With and without.
Result	:	Negative.
Method	:	OECD Guidelines for the Testing of Chemicals, Number 471, May 1983: "Genetic Toxicology: *Salmonella Typhimurium* Reverse Mutation Assay"
Year	:	1991
GLP	:	Yes.
Method	:	The test compound was evaluated in triplicate cultures in strains TA1535, TA1537, TA1538, TA98 and TA100 in the presence and absence of S9 at doses of 10, 100, 1,000, 2,500 and 5,000 µg/plate.
Result	:	No toxicity was observed in the background lawn. The ratio of revertants in treated plates versus controls never exceeded 1.6. No significant increase in mutations either in presence or absence of S-9.
Test substance	:	ADAMMC (80% solution in water)
Conclusion	:	ADAMMC was not mutagenic in this *in vitro* assay.
Reliability	:	(1) valid without restrictions Guideline study.

06.11.2003 (14)

Type	:	Cytogenetic assay.
Reference		Adams, K. (1990)
System of testing	:	Human lymphocytes.
Test concentration	:	0 – 3,000 µg/plate
Metabolic activation	:	With and without.
Result	:	Negative.
Method	:	OECD Guidelines for the Testing of Chemicals, Number 473, 1983: "Genetic Toxicology: *In Vitro* Mammalian Cytogenetic Test".
Year	:	1990.
GLP	:	Yes.
Method	:	Human blood was collected, washed 3 times and suspended at a concentration of $1x10^6$ cells. 5ml-aliquots were incubated at 37°C for 48 hours. Test compound was added to give final concentration of 9.8, 19.5, 39.1, 78.2, 156, 313, 625, 1,250, 2,500 and 5,000 µg/ml (positive and negative controls were used). For metabolic activation 1.25 ml S9 was added to each culture. Cultures were incubated for 24 hours (2 hour exposure). Colchine was added to each culture. After 2 hours, cells were centrifuged, collected and fixed. Slides were stained using Giemsa solution. Metaphase figures were identified and chromosomes analyzed.
Result	:	While a small increase in chromosomal damage was seen at the highest dose this increase, 2.5% aberrant cells fell within historical control range and was not considered to be indicative of clastogenic activity. No compound-related effect was seen in the presence of metabolic activation.
Test substance	:	ADAMMC (80% solution in water)
Conclusion	:	ADAMMC was not clastogenic in this *in vitro* assay.
Reliability	:	(1) valid without restrictions Guideline study.

06.11.2003 (15)

Type	:	Mammalian cell gene mutation assay.
Reference		Wollny, H-E. (1997).
System of testing	:	Mouse lymphoma ($TK^{+/-}$) L5178Y cells
Test concentration	:	30 – 3,000 µg/plate
Metabolic activation	:	With and without.
Result	:	Negative.
Method	:	OECD Guidelines for the Testing of Chemicals, Number 476, April 4, 1984: "Genetic Toxicology: *In Vitro* Mammalian Cell Gene Mutation Test"
Year	:	1997
GLP	:	Yes.
Method	:	Cells were suspended in medium with test article in the presence or absence of S9 metabolic activation for 4 hours. Article was removed by centrifugation and cells washed twice. Cells were plated to determine cell density (cloning efficiency). Cells were selected in the presence of 100 µg/ml TFT after 14 days.
Result	:	The highest concentration applied produced a decrease of cell culture growth and the cell growth observed at the lowest concentration was approximately in the range of the negative control. No precipitation of test article was observed. No substantial and reproducible increase in mutant colony numbers was observed at any valuated concentration neither in the presence or absence of metabolic activation. Furthermore, there was no indication of a dose-dependant increase in the number of spontaneous mutant colonies in the solvent control. In this study the range of negative controls was from 31 up to 47 mutant colonies per 10^6 cells; the range of groups treated with test article was from 29 up to 68 mutant colonies per 10^6 cells.
Test substance	:	ADAMMC (80% solution in water)
Conclusion	:	ADAMMC did not demonstrate mutagenic potential in this *in vitro* assay.
Reliability	:	(1) valid without restrictions Guideline study.

07.11.2003 (16)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 OTHER RELEVANT INFORMATION

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS OF HANDLING AND STORING

Avoid all contact with the product by ingestion, inhalation or contact with the skin, eyes and clothing. Do not breathe vapors or spray mist. Wash hands and face before breaks and immediately after handling the product. When using, do not smoke. Handle in accordance with good industrial hygiene and safety practice.
Store in contact with air. Do not exceed storage temperature of 30°C. Protect from light.
05.11.2003

8.2 FIRE GUIDANCE

This product does not burn in aqueous solution. No special precautions required. In case of fire, wear a self contained breathing apparatus. Keep containers cool during fire with water spray.
05.11.2003

8.3 EMERGENCY MEASURES

If product is inhaled, move to fresh air.
In case of skin contact, rinse and wash contaminated clothing before re-use. Wash contaminated area immediately for at least 15 minutes. In case of persistent skin irritation, consult a physician.
In case of eye contact, rinse immediately with plenty of water for at least 15 minutes. Keep eye wide open while rinsing and lift upper and lower ids to ensure complete removal of chemical. In case of persistent eye irritation, consult a physician.
If swallowed, do not induce vomiting. Rinse mouth (never give anything by mouth to an unconscious person). Call a physician immediately.
In case of accidental release, do not allow product to enter drains. Do not contaminate water. Dam up spills. Soak with inert absorbent material. If liquid has been spilled in large quantities, clean up promptly by scoop or vacuum. Keep in suitable and closed containers for disposal. After cleaning, flush area with water.
05.11.2003

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

Not applicable.
05.11.2003

8.5 WASTE MANAGEMENT

Can be land filled or incinerated when in compliance with local regulations.
05.11.2003

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Wehrhahn, D. (1999a) Inherent Biodegradability Modified Zahn-Wellens Test. Stockhausen GmbH and Co. KG, Laboratory for Toxicology and Ecology, Krefeld, Germany

(2) Calmels, R. (1994a). Test to evaluate acute toxicity (96 hours) in freshwater fish (*Brachydanio rerio*) using a static method – ADAM MeCl. Société d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

(3) Wehrhahn, D. (1999) Acute Fish Toxicity of Adam-Quat on *Danio rerio* (Zebra Fish). Stockhausen GmbH and Co. KG, Laboratory for Toxicology and Ecology, Krefeld, Germany

(4) Calmels, R. (199b4). Test to Evaluate Acute Toxicity(48 hours) in Daphnia – ADAM MeCl. Société d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

(5) Wehrhahn, D. (1999b) Acute Daphnia Toxicity of Adame-Quat on *Daphnia magna*. Stockhausen GmbH and Co. KG, Laboratory for Toxicology and Ecology, Krefeld, Germany

(6) Licata-Messana, L. (1994). Inhibition Test (72 hours) in Freshwater Unicellular Algae - ADAM MECL. Société d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

(7) Wehrhahn, D. (1999c) Chronic Alga Toxicity of Adame-Quat on *Scendedesmus subspicatus*. Stockhausen GmbH and Co. KG, Laboratory for Toxicology and Ecology, Krefeld, Germany

(8) Wehrhahn, D. (1999d) Chronic Bacteria Toxicity of Adame-Quat on *Psuedomonas putida*. Stockhausen GmbH and Co. KG, Laboratory for Toxicology and Ecology, Krefeld, Germany

(9) Clouzeau, J. (1990). ADQUAT MC 80 Evaluation de la toxicité aiguë par voie orale chez le rat. Centre International de Toxicologie (CIT), Miserey, France

(10) Collier, T.A. (1985a). Range Finding Oral Toxicity Test: An Assessment of the Acute Oral Toxicity of ADQUAT 80 MC in the Rat, Safepharm Laboratories, Derby, UK.

(11) Collier, T.A. (1985b). OECD Skin Irritation Test: Determination of the Degree of Primary Cutaneous Irritation Caused by ADQUAT 80 MC in the Rabbit. Safepharm Laboratories, Derby, UK.

(12) Collier, T.A. (1985c). OECD Eye Irritation Test: Determination of the Degree of Ocular Irritation Caused by ADQUAT 80 MC in the Rabbit. Safepharm Laboratories, Derby, UK.

(13) Collier, T.A. (1985d). Magnusson & Klugman Maximization Study: Determination of the Contact Sensitization Potential of ADQUAT 80 MC in the Guinea Pig. Safepharm Laboratories, Derby, UK.

(14) Clouzeau, J. (1991). Acryloxyethyltrimethylammonium Chloride (80% Solution in Water) (ADAMQUAT MC 80) - Reverse Mutation Assay by the Ames Test. Centre International de Toxicologie (CIT), Miserey, France,

(15) Adams, K. (1990). ADAMQUAT MC 80: Metaphase Chromosome Analysis of Human Lymphocytes Cultured *In Vitro*. Huntington Laboratories, Cambridgeshire, UK.

(16) Wollny, H-E. (1997). Cell Mutation Assay at the Thymidine Kinase ($TK^{+/-}$) Locus in Mouse Lymphoma L5178Y Cells with DMAEA.MCQ Monomer. RCC, Rossdorf, Germany.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-15210B1

IUCLID

Data Set

Existing Chemical	:	Substance ID: 13106-44-0
CAS No.	:	13106-44-0
TSCA Name	:	Ethanaminium, *N*,*N*,*N*-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, methyl sulfate
Structural formula	:	CH2=CHCOOC2H4N(CH3)3.CH3SO4
Molecular formula	:	C7H16NO6S
Molecular weight	:	269.32
Producer related part		
Company	:	Quat HPV Challenge Task Group
Creation date	:	03.11.2003
Substance related part		
Company	:	Quat HPV Challenge Task Group
Creation date	:	03.11.2003
Number of pages	:	22
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	Organic.
Physical status	:	Solid.
Purity	:	> 99%.
Remark	:	The commercial product is manufactured and shipped as a solution (75 – 80%) in water.

03.11.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Dimethylaminoethylacrylate, dimethyl sulfate
03.11.2003

Dimethylaminoethyl acrylate methyl sulfate
03.11.2003

[2-(acryloyloxy)ethyl]trimethylammonium methyl sulfate
03.11.2003

[(Acryyloxy)ethyl]trimethylammonium methyl sulfate
03.11.2003

ADAM DMS
03.11.2003

DMAEA DMS
03.11.2003

1.3 IMPURITIES

Dimethylaminoethylacrylate (<0.1%).
04.11.2003

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

Sensitizing. Irritating to eyes.
04.11.2003

1.6.2 CLASSIFICATION

Not Regulated
04.11.2003

1.6.3 PACKAGING

1.7 USE PATTERN

Type	:	Industrial
Category	:	Chemical industry; used in synthesis of water soluble polymers, flocculants, retention aids.
Remark	:	Commercial product is manufactured and shipped as a solution in water (75–80%).

04.11.2003

1.7.1 DETAILED USE PATTERN

Type	:	Industrial.
Category	:	Chemical industry; used in synthesis.
Remark	:	Water-soluble polymers. Flocculants. Retention aids.

04.11.2003

1.7.2 METHODS OF MANUFACTURE

Manufactured by reaction of dimethyl sulfate with dimethylaminoethylacrylate.
04.11.2003

1.8 REGULATORY MEASURES

None

04.11.2003

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

None
04.11.2003

1.8.2 ACCEPTABLE RESIDUES LEVELS

Dimethylaminoethyacrylate (ADAM) at less than 0.1%.
04.11.2003

1.8.3 WATER POLLUTION

Not applicable
04.11.2003

1.8.4 MAJOR ACCIDENT HAZARDS

Not applicable
04.11.2003

1.8.5 AIR POLLUTION

Not applicable
04.11.2003

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

Listed on all major chemical inventories (TSCA, EINECS, ECL, AICS, etc.).
04.11.2003

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

Not applicable
04.11.2003

1.9.2 COMPONENTS

Pure substance (in aqueous solution).
04.11.2003

1.10 SOURCE OF EXPOSURE

None
04.11.2003

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

2.1 MELTING POINT

Value	:	=211.70°C.
Method	:	MPBPWIN v1.40.
Year	:	2003.
GLP	:	No.
Test substance	:	ADAMDMS (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

05.11.2003

2.2 BOILING POINT

Value	:	=498.07°C
Method	:	MPBPWIN v1.40 (adapted Stein & Brown method).
Year	:	2003.
GLP	:	No.
Test substance	:	ADAMDMS (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

05.11.2003

2.3 DENSITY

Type	:	Density
Value	:	= 1.12 g/cm3 at 20°C
Method	:	other: no data
Year	:	no data
GLP	:	no data
Test substance	:	ADAMDMS(80% solution in water)
Reliability	:	(4) not assignable Only short information available (safety data sheet)

05.11.2003

2.3.1 GRANULOMETRY

Not applicable.
05.11.2003

2.4 VAPOUR PRESSURE

Value	:	=3.18 E-10 mm Hg at 25°C
Method	:	MPBPWIN v1.40 (modified Grain method).
Year	:	2003.
GLP	:	No.
Test substance	:	ADAMDMS (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

05.11.2003

2.5 PARTITION COEFFICIENT

Partition coefficient	:	Octanol-water.
log Pow	:	= -1.40
Method	:	KOWWIN v1.66.
Year	:	2003
GLP	:	No.
Test substance	:	ADAMDMS (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

05.11.2003

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water.
Value	:	Completely miscible.
Method	:	Other: no data.
GLP	:	No data.
Test substance	:	ADAMDMS (pure substance)
Reliability	:	(4) not assignable. Only short information available (safety data sheet).

05.11.2003

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

Value	:	30-50 mPa.s
Method	:	Other: no data.

GLP	:	No data.
Test substance	:	ADAMDMS (80%).
Reliability	:	(4) not assignable. Only short information available (safety data sheet).

04.11.2003

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	Air.
Method	:	AOPWIN v1.90.
Year	:	2003.
GLP	:	No.
Result	:	The atmospheric degradation behavior was assessed using AOPWIN (v. 1.90). An overall OH rate constant of 25.6167 E-12 cm^3/molecule.sec was obtained. The following half-lives can be predicted under the chosen conditions: 0.418 days (12h-day, 1.5 E6 OH/cm^3); 5.010 hours. Overall ozone rate constant = 0.175 E-17 cm^3/molecule-sec. Half-life = 6.549 days (at 7 E11 mol/ cm^3)
Test substance	:	ADAMDMS (pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

05.11.2003

3.1.2 STABILITY IN WATER

Type	:	Abiotic (hydrolysis).
Method	:	HYDROWIN v1.67
Year	:	2003.
GLP	:	No.
Remark	:	The estimated hydrolysis half-life of this substance at: pH 7 = 9.001 years; ph 8 = 328.762 days
Test substance	:	ADAMDMS (pure substance)
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

05.11.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	Volatility.
Media	:	Water – air.
Method	:	HENRYWIN v3.10.
Year	:	2003.
Remark	:	The value obtained for for Henry's constant was calculated as: Bond contribution method: 7.01 E-19 atm-m^3/mole (group contribution calculation incomplete). According to Thomas (1990), the substance may be considered as "not volatile from water".

Henry's LC (VP/WSol estimate using EPI values) = 1.353 E-13 atm-m^3/mole

Test substance : ADAMDMS (pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

05.11.2003

Type : Level III Fugacity Model
Media : Water – air – soil – sediment.
Method : BCFWIN v2.14.
Year : 2003.
Result : The value obtained from the Level III Fugacity Model are as follows:

	Mass Amount (%)	Half-Life (hr)	Emissions (kg/hr)
Air	5.01 E-10	9.42	1000
Water	49.8	900	1000
Soil	50.1	900	1000
Sediment	0.0918	3.6 E3	0

Persistence time = 789 hours.

Conclusion : Regardless of the media to which ADAMMC is released, virtually all at steady state is in the soil and water phases. Using the default emissions of equal amounts to soil, air, water and sediment (1000 kg/hr for each) the Level III model predicts that the distribution of ADAMMC will be 50.1% in soil, 49.8% in water, <0.1% in sediment, and virtually nothing in air.
Test substance : ADAMDMS (pure substance)
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

3.3.2 DISTRIBUTION

Media : air – biota – sediment(s) – soil – water
Method : calculation according to Mackay, Level 1
Year : no data
Remark : The following parameters were employed in this calculation:

vapor pressure:	1.8 E-5 Pa	(20°C)	(calculated)
molecular weight:	207.7 g/mol		
water solubility:	ca. 6000 g/l	(20°C)	(calculated)
logPow:	–2.55	(25°C)	(calculated)

Result : The following environmental distribution was predicted:
water: ca. 100%, other environmental compartments below 0.001%
Reliability : (2) valid with restrictions
Generally accepted method of calculation with restrictions

04.11.2003

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : Static.
Species : *Brachydanio rerio* (Zebra fish) (Fish, fresh water).
Reference Calmels, R. (1994a).
Exposure period : 96 hours
Unit : mg/l
LC0 : > 100
LC50 : Not observed.
LC50 : Not observed.
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 203, 1984: "Fish, Acute Toxicity Test".
Year : 1994
GLP : No.
Test substance : ADAMEDMS
Test procedure : Groups of 10 fresh water Zebra fish (*Brachydanio rerio*) were exposed in a reconstituted medium at 23° C for 96 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Fish mortality was measured after 24, 48 and 96 hours.

Results :

	Mortality		
Test Concentration (mg/L)	24 hours	48 hours	96 hours
0	0	0	0
1	0	0	0
10	0	0	0
100	0	0	0

Since the LC0 at 24, 48 and 96 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : ADAMDMS (80% solution in water)
Conclusion : ADAMDMS (80% solution in water) is not toxic to freshwater fish at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

03.11.2003 (1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : Static.
Reference Calmels, R. (1994b).
Species : *Daphnia magna* (Crustacean, fresh water)
Exposure period : 48 hours.
Unit : mg/l
EC0 (immobilization) : > 100
EC50 (immobilization) : Not observed.
EC100 (immobilization) : Not observed.
Analytical monitoring : No.

Method : OECD Guidelines for the Testing of Chemicals, No. 202, April 1984: "*Daphnia* sp., Acute Immobilization Test".
Year : 1994
GLP : No.
Test substance : ADAME DMS
Test procedure : Groups of 10 fresh water daphnia (*Daphnia magna*) were exposed in a reconstituted medium at 23° C for 48 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Immobilized daphnia were counted after 24 and 48 hours.
Results :

		Immobilization		
Concentration (mg/L)	No. of daphnia	No. after 24 hours	No. after 48 hours	% after 48 hours
0	20	0	1	5
1	20	0	1	5
10	20	0	0	0
100	20	0	0	0

Since the EC50 at 24 and 48 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : ADAMDMS (80% solution in water)
Conclusion : ADAMDMS (80% solution in water) has no effect on the swimming behavior of daphnia at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

03.11.2003 (2)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Type : Static.
Reference Licata-Messana, L. (1994).
Species : *Scenedesmus subspicatus* (Algae, unicellular, fresh water)
Exposure period : 72 hours
Unit : mg/l
EC_A50 (l) : $1<EC_A<10$
$EC_\mu50$ (l) : >100
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 201, June 1984: "Alga, Growth Inhibition Test".
Year : 1994
GLP : No.
Test substance : ADAME DMS
Test procedure : Blue-green algae (*Scenedesmus subspicatus*) were exposed in a reconstituted medium at 23° C for 72 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Algal concentrations were measured after 24, 48 and 72 hours.

Results :

	Algal Concentration				
Concentration (mg/L)	Start	24 hours	48 hours	72 hours	% growth inhibition
0	10,000	103,472	725,000	2,867,361	0
1	10,000	61,111	487,509	2,547,222	2
10	10,000	29,267	50,000	256,944	43
100	10,000	20,833	18,056	20,833	87

The test was terminated after the range-finding phase.

Test substance : ADAMDMS (80% solution in water).
Conclusion : ADAMDMS (80% solution in water) significantly inhibits algal growth at concentrations greater than10 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

03.11.2003 (3)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 OTHER RELEVANT INFORMATION

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS OF HANDLING AND STORING

Avoid all contact with the product by ingestion, inhalation or contact with the skin, eyes and clothing. Do not breathe vapors or spray mist. Wash hands and face before breaks and immediately after handling the product. When using, do not smoke. Handle in accordance with good industrial hygiene and safety practice.
Store in contact with air. Do not exceed storage temperature of 30°C. Protect from light.
04.11.2003

8.2 FIRE GUIDANCE

This product does not burn in aqueous solution. No special precautions required. In case of fire, wear a self contained breathing apparatus. Keep containers cool during fire with water spray.
04.11.2003

8.3 EMERGENCY MEASURES

If product is inhaled, move to fresh air.
In case of skin contact, rinse and wash contaminated clothing before re-use. Wash contaminated area immediately for at least 15 minutes. In case of persistent skin irritation, consult a physician.
In case of eye contact, rinse immediately with plenty of water for at least 15 minutes. Keep eye wide open while rinsing and lift upper and lower ids to ensure complete removal of chemical. In case of persistent eye irritation, consult a physician.
If swallowed, do not induce vomiting. Rinse mouth (never give anything by mouth to an unconscious person). Call a physician immediately.
In case of accidental release, do not allow product to enter drains. Do not contaminate water. Dam up spills. Soak with inert absorbent material. If liquid has been spilled in large quantities, clean up promptly by scoop or vacuum. Keep in suitable and closed containers for disposal. After cleaning, flush area with water.
04.11.2003

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

Not applicable.
04.11.2003

8.5 WASTE MANAGEMENT

Can be land filled or incinerated when in compliance with local regulations.
04.11.2003

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Calmels, R. (1994a). Test to Evaluate Acute Toxicity (96hours) in Freshwater Fish (*Brachydanio rerio)* Using a static Method ADAME DMS. Societe d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

(2) Calmels, R. (1994b). Test to Evaluate Acute Toxicity (48hours) in Daphnia ADAME DMS. Societe d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

(3) Licata-Messana, L. (1994). Inhibition Test (72 hours) in Freshwater Unicellular Algae ADAME DMS. Societe d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

IUCLID

Data Set

Existing Chemical	:	Substance ID: 5039-78-1
CAS No.	:	5039-78-1
TSCA Name	:	Dimethylaminoethylmethacrylate, methyl chloride
Structural formula	:	CH2=C(CH3)COOC2H4N(CH3)3.Cl
Molecular formula	:	C9H18NO2.Cl

Producer related part

Company	:	Quat HPV Challenge Task Group
Creation date	:	12.11.2003

Substance related part

Company	:	Quat HPV Challenge Task Group
Creation date	:	12.11.2003

Number of pages	:	23
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	Organic.
Physical status	:	Solid.
Purity	:	> 99%.
Remark	:	The commercial product is manufactured and shipped as a solution (75 – 80%) in water.

12.11.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Ethanaminium, *N*, *N*, *N*-trimethyl-2[(2-methyl-1oxo-2-propenyl)oxy]-, chloride
12.11.2003

2-Trimethylammoniumethyl methacrylate chloride
12.11.2003

Choline chloride methacrylate
12.11.2003

Dimethylaminoethyl methacrylate methochloride
12.11.2003

N, N, N-Trimethyl-2-[(2-methyl-1-oxo-2-propenyl)oxy]ethanaminium chloride
12.11.2003

Trimethylammoniuomethyl methacrylate chloride
12.11.2003

[2-(Methacryloyloxy)ethyl]trimethylammonium chloride
12.11.2003

[(Methacryyloxy)ethyl]trimethylammonium chloride
12.11.2003

MADAM MC
12.11.2003

DMAEM MC
12.11.2003

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type	:	Industrial
Category	:	Chemical industry; used in synthesis of water soluble polymers, flocculants, retention aids.
Remark	:	Commercial product is manufactured and shipped as a solution in water (75–80%).

12.11.2003

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10SOURCE OF EXPOSURE

1.11ADDITIONAL REMARKS

1.12LAST LITERATURE SEARCH

1.13REVIEWS

2.1 MELTING POINT

Value	:	=151.81°C.
Method	:	MPBPWIN v1.40.
Year	:	2003.
GLP	:	No.
Test substance	:	MADAMMC (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

12.11.2003

2.2 BOILING POINT

Value	:	=405.99°C
Method	:	MPBPWIN v1.40 (adapted Stein & Brown method).
Year	:	2003.
GLP	:	No.
Test substance	:	MADAMMC (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

12.11.2003

2.3 DENSITY

Type	:	density
Value	:	= 1.18 g/cm3 at 25°C (80% solution in water).
Method	:	other: no data
Year	:	no data
GLP	:	no data
Test substance	:	MADAM MC (80% solution in water)
Reliability	:	(4) not assignable Only short information available (safety data sheet)

12.11.2003 (1)

2.3.1 GRANULOMETRY

Not applicable.
12.11.2003

2.4 VAPOUR PRESSURE

Value	:	=3.03 E-7 mm Hg at 25°C
Method	:	MPBPWIN v1.40 (modified Grain method).
Year	:	2003.
GLP	:	No.
Test substance	:	MADAMMC (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

12.11.2003

2.5 PARTITION COEFFICIENT

Partition coefficient	:	Octanol-water.
log Pow	:	-2.55
Method	:	KOWWIN v1.66.
Year	:	2003
GLP	:	No.
Test substance	:	MADAMMC (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

13.11.2003

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water.
Value	:	Completely miscible.
Method	:	Other: no data.
GLP	:	No data.
Test substance	:	MADAMMC (pure substance)
Reliability	:	(4) not assignable. Only short information available (safety data sheet).

13.11.2003

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	Does not flash.
Method	:	Other: no data.
Year	:	No data.
GLP	:	No data.
Test substance	:	MADAM MC (80% solution in water).
Reliability	:	(4) not assignable Only short information available (safety data sheet)

13.11.2003

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

Value	:	100 mPa.s
Method	:	Other: no data.
GLP	:	No data.
Test substance	:	MADAMMC (80%).
Reliability	:	(4) not assignable. Only short information available (safety data sheet).

13.11.2003

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	Air.
Method	:	AOPWIN v1.90.
Year	:	2003.
GLP	:	No.
Result	:	The atmospheric degradation behavior was assessed using AOPWIN (v.1.90). An overall OH rate constant of 34.4425 E-12 cm^3/molecule.sec was obtained. The following half-lives can be predicted under the chosen conditions: 0.311 days (12h-day, 1.5 E6 OH/cm^3); 3.727 hours. Overall ozone rate constant = 0.175 E-17 cm^3/molecule-sec. Half-life = 1.007 days (at 7 E11 mol/ cm^3)
Test substance	:	MADAMMC (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

13.11.2003

3.1.2 STABILITY IN WATER

Type	:	Abiotic (hydrolysis).
Method	:	HYDROWIN v1.67
Year	:	2003.
GLP	:	No.
Remark	:	The estimated hydrolysis half-life of this substance at: pH 7 = 68.343 years; pH 8 = 6.834 years
Test substance	:	MADAMMC (100% pure substance).
Reliability	:	(2) valid with restrictions. Generally accepted method of calculation with restrictions.

13.11.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	Volatility.
Media	:	Water – air.
Method	:	HENRYWIN v3.10.
Year	:	2003.
Remark	:	The value obtained for for Henry's constant was calculated as: Bond contribution method: 1.09 E-14 atm-m^3/mole (group contribution calculation incomplete). According to Thomas (1990), the substance may

be considered as "not volatile from water".
Henry's LC (VP/WSol estimate using EPI values) = 8.281 E-14 atm-m^3/mole

Test substance : MADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

14.11.2003

Type : Level III Fugacity Model
Media : Water – air – soil – sediment.
Method : BCFWIN v2.14.
Year : 2003.
Result : The value obtained from the Level III Fugacity Model are as follows:

	Mass Amount (%)	Half-Life (hr)	Emissions (kg/hr)
Air	4.12 E-7	5.7	1000
Water	45.3	360	1000
Soil	54.6	360	1000
Sediment	0.0755	1.44 E3	0

Persistence time = 421 hours.

Conclusion : Regardless of the media to which MADAMMC is released, virtually all at steady state is in the soil and water phases. Using the default emissions of equal amounts to soil, air, water and sediment (1000 kg/hr for each) the Level III model predicts that the distribution of MADAMMC will be 54.6% in soil, 45.3% in water, <0.1% in sediment, and virtually nothing in air.

Test substance : MADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

14.11.2003

3.3.2 DISTRIBUTION

Media : air – biota – sediment(s) – soil – water
Method : calculation according to Mackay, Level 1
Year : no data
Remark : The following parameters were employed in this calculation:

vapor pressure:	1.8 E-5 Pa	(20°C)	(calculated)
molecular weight:	207.7 g/mol		
water solubility:	ca. 6000 g/l	(20°C)	(calculated)
logPow:	–2.55	(25°C)	(calculated)

Result : The following environmental distribution was predicted:
water: ca. 100%, other environmental compartments below 0.001%
Reliability : (2) valid with restrictions
Generally accepted method of calculation with restrictions

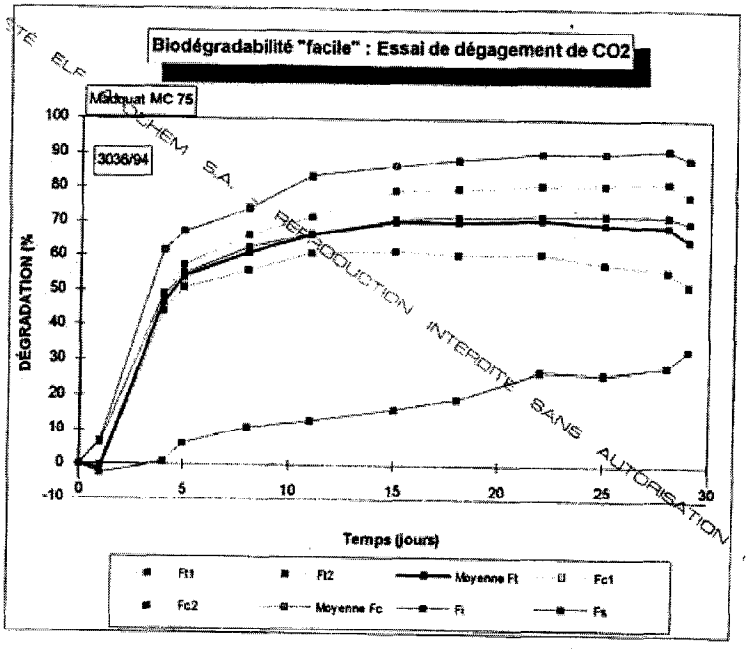
14.11.2003

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : Aerobic.
Reference : Thiébaud, H. (1994).

Inoculum	:	WWTP effluent.
Concentration	:	48.7 mg/l (corresponding to a DOC of 20 mg/l)
Contact time	:	28 days
Degradation	:	= 71% after 22 days (plateau) = 69% after 28 days
Result	:	Readily biodegradable.
Deg. Product	:	Not measured.
Method	:	OECD Guidelines for the Testing of Chemicals, No. 301B, July 17, 1992: "Ready Biodegradability: Modified Sturm Test (CO2 evolution)".
Year	:	1994
GLP	:	Yes.
Test substance	:	MADAMMC (75% solution in water).
Remark	:	The test substance is referred to as MADQUAT MC 75
Method	:	Biodegradation of MADAM MC by an inoculum of $1.22X10^5$ bacterium from the secondary treatment at Versailles (France) MWWTP was determined at 22°C. Percentage of CO2 produced was determined after collection in NaOH.
Result	:	The maximum level of biodegradation attained was 71% after 22 days. The lag period for degradation of the test material (time from start of study until 10% degradation) was less than 5 days and the degradation 10 days after the lag period was 70%. The study met all the required validity criteria. The graphical representation of the biodegradation is shown below:



Test substance	:	MADAMMC (75% solution in water)
Conclusion	:	MADAMMC was considered to be readily biodegradable
Reliability	:	(1) valid without restrictions Guideline study.

14.11.2003 (1)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : Static
Reference Calmels, R. (1994a).
Species : *Brachydanio rerio* (Zebra fish)(Fish, fresh water).
Exposure period : 96 hours.
Unit : mg/l
LC0 : > 100
LC50 : Not observed.
LC50 : Not observed.
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 203, 1984: "Fish, Acute Toxicity Test".
Year : 1994.
GLP : No.
Test substance : MADAME MECL
Test procedure : Groups of 10 fresh water Zebra fish (*Brachydanio rerio*) were exposed in a reconstituted medium at 23° C for 96 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Fish mortality was measured after 24, 48 and 96 hours.

Results :

	Mortality		
Test Concentration (mg/L)	24 hours	48 hours	96 hours
0	0	0	0
1	0	0	0
10	0	0	0
100	0	0	0

Since the LC0 at 24, 48 and 96 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : MADAMMC (80% solution in water)
Conclusion : MADAMMC (80% solution in water) is not toxic to freshwater fish at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

13.11.2003 (2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : Static
Reference Calmels, R. (1994b).
Species : *Daphnia magna* (Crustacean, fresh water)
Exposure period : 48 hours.
Unit : mg/l
EC0 (immobilization) : > 100.
EC50 (immobilization) : Not observed.
EC100 (immobilization) : Not observed.
Analytical monitoring : No.

Method : OECD Guidelines for the Testing of Chemicals, No. 202, April 1984: "*Daphnia* sp., Acute Immobilization Test".
Year : 1994.
GLP : No
Test substance : MADAME MECL
Test procedure : Groups of 10 fresh water daphnia (*Daphnia magna*) were exposed in a reconstituted medium at 23° C for 48 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Immobilized daphnia were counted after 24 and 48 hours.
Results :

		Immobilization		
Concentration (mg/L)	No. of daphnia	No. after 24 hours	No. after 48 hours	% after 24 hours
0	20	0	1	5
1	20	0	1	5
10	20	0	0	0
100	20	0	0	0

Since the EC50 at 24 and 48 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : MADAMMC (80% solution in water)
Conclusion : MADAMMC (80% solution in water) has no effect on the swimming behavior of daphnia at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

13.11.2003 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Type : Static
Reference Licata-Messana, L. (1994).
Species : *Scenedesmus subspicatus* (Algae, unicellular, fresh water).
Exposure period : 72 hours.
Unit : mg/l
EC_A50 (I) : Not observed.
$EC_\mu50$ (I) : Not observed.
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 201, June 1984: "Alga, Growth Inhibition Test".
Year : 1994
GLP : No
Test substance : MADAME MECL
Test procedure : Blue-green algae (*Scenedesmus subspicatus*) were exposed in a reconstituted medium at 23° C for 72 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Algal concentrations were measured after 24, 48 and 72 hours.

Results :

Concentration (mg/L)	Algal Concentration				% growth inhibition
	Start	24 hours	48 hours	72 hours	
0	10,000	25,965	165,972	820,833	0
1	10,000	50,000	126,399	899,611	-4
10	10,000	50,000	159,722	754,167	2
100	10,000	62,500	95,834	584,722	26

Since both the EC_A50 and the $EC_\mu50$ at 24, 48 and 72 hours were greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : MADAMMC (80% solution in water)
Conclusion : MADAMMC (80% solution in water) does not significantly inhibit algal growth at 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

13.11.2003 (4)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test.
Reference		Molinier, B. (1992).
System of testing	:	*Salmonella typhimurium* TA1535, TA1537, TA1538, TA98 and TA100
Test concentration	:	312.5 – 5000 ug/plate
Metabolic activation	:	With and without S9.
Result	:	Negative
Method	:	OECD Guidelines for the Testing of Chemicals, No. 471 "Genetic Toxicology: *Salmonella typhimurium* Reverse Mutation Assay".
Year	:	1992
GLP	:	Yes.
Test substance	:	MADAMMC (75% solution in water)
Method		The test compound was evaluated in triplicate cultures in strains TA1535, TA1537, TA1538, TA98 and TA100 in the presence and absence of S9 at the above doses. (Ames *et al*, 1975)
Result		The ratio of revertants in treated plates versus controls never exceeded 1.4. No significant increase in mutations either in presence or absence of S-9.
Test substance	:	MADAMMC (75% solution in water)
Conclusion	:	MADAMMC was not mutagenic in this in vitro assay.
Reliability	:	(1) valid without restrictions Guideline study.

13.11.2003

(5)

Type	:	Cytogenetic assay
Reference		Molinier, B. (1995).
System of testing	:	Human lymphocytes
Test concentration	:	625, 1250, 2,500 and 5,000 µg/ml.
Metabolic activation	:	With and without.
Result	:	Negative.
Method	:	OECD Guidelines for the Testing of Chemicals, No. 473: "*In Vitro* Mammalian Chromosome Aberration Test".
Method	:	Human blood was collected, washed 3 times and suspended at a concentration of $1x10^6$ cells. 5ml-aliquots were incubated at 37°C for 48 hours. Test compound was added to give final concentration of 625, 1250, 2,500 and 5,000 µg/ml (positive and negative controls were used). For metabolic activation 1.25 ml S9 was added to each culture. Cultures were incubated for 24 hours (2 hour exposure). Colchicine was added to each culture. After 2 hours, cells were centrifuged, collected and fixed. Slides were stained using Giemsa solution. Metaphase figures were identified and chromosomes analyzed.
Result		No significant increase in chromosomal damage was seen at any dose tested. No compound-related effect was seen in the presence of metabolic activation.
Year	:	1995.
GLP	:	Yes.
Test substance	:	MADAMMC (75% solution in water)
Conclusion	:	MADAMMC was not clastogenic in this in vitro assay.
Reliability	:	(1) valid without restrictions Guideline study.

13.11.2003 (6)

Type	:	Mammalian cell gene mutation assay
Reference		Adams, K. (1997).
System of testing	:	Mouse lymphoma ($T/K^{+/-}$) L5178Y cells
Test concentration	:	300 – 5000 ug/plate
Method		OECD Guidelines for the Testing of Chemicals, No. 476 "Genetic Toxicology: *In vitro* Mammalian Cell Gene Mutation Test".
Metabolic activation	:	With and without (S9).
Result	:	Negative.
Year	:	1997
GLP	:	Yes.
Method	:	Cells were suspended in medium with test article in the presence or absence of S9 metabolic activation for 4 hours. Article was removed by centrifugation and cells washed twice. Cells were plated to determine cell density (cloning efficiency). Cells were selected in the presence of 100 µg/ml TFT after 14 days.
Result		The highest concentration applied produced a decrease of cell culture growth and the cell growth observed at the lowest concentration was approximately in the range of the negative control. No precipitation of test article was observed. No substantial and reproducible increase in mutant colony numbers was observed at any valuated concentration neither in the presence or absence of metabolic activation. Furthermore, there was no indication of a dose-dependant increase in the number of spontaneous mutant colonies in the solvent control. The material did not significantly increase the mutant frequency in this test.
Test substance	:	MADAMMC (75% solution in water)
Conclusion	:	MADAM MC did not demonstrate mutagenic potential in this *in vitro* assay.
Reliability	:	(1) valid without restrictions Guideline study.

13.11.2003 (7)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 OTHER RELEVANT INFORMATION

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS OF HANDLING AND STORING

Avoid all contact with the product by ingestion, inhalation or contact with the skin, eyes and clothing. Do not breathe vapors or spray mist. Wash hands and face before breaks and immediately after handling the product. When using, do not smoke. Handle in accordance with good industrial hygiene and safety practice.
Store in contact with air. Do not exceed storage temperature of 30°C. Protect from light.
14.11.2003

8.2 FIRE GUIDANCE

This product does not burn in aqueous solution. No special precautions required. In case of fire, wear a self contained breathing apparatus. Keep containers cool during fire with water spray.
14.11.2003

8.3 EMERGENCY MEASURES

If product is inhaled, move to fresh air.
In case of skin contact, rinse and wash contaminated clothing before re-use. Wash contaminated area immediately for at least 15 minutes. In case of persistent skin irritation, consult a physician.
In case of eye contact, rinse immediately with plenty of water for at least 15 minutes. Keep eye wide open while rinsing and lift upper and lower ids to ensure complete removal of chemical. In case of persistent eye irritation, consult a physician.
If swallowed, do not induce vomiting. Rinse mouth (never give anything by mouth to an unconscious person). Call a physician immediately.
In case of accidental release, do not allow product to enter drains. Do not contaminate water. Dam up spills. Soak with inert absorbent material. If liquid has been spilled in large quantities, clean up promptly by scoop or vacuum. Keep in suitable and closed containers for disposal. After cleaning, flush area with water.
14.11.2003

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

Not applicable.
14.11.2003

8.5 WASTE MANAGEMENT

Can be land filled or incinerated when in compliance with local regulations.
14.11.2003

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Thiébaud, H. (1994). MADQUAT MC 75 - Détermination de la Biodégradabilité Facile. Essai de Dégagement de CO2. Elf-Atochem, Centre d'Application de Levallois-Perret, Levallois, France.

(2) Calmels, R. (1994a). Test to Evaluate Acute Toxicity (96hours) in Freshwater Fish (*Brachydanio rerio)* Using a static Method MADAM MECL. Societe d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

(3) Calmels, R. (1994b). Test to Evaluate Acute Toxicity (48hours) in Daphnia MADAM MECL. Societe d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

(4) Licata-Messana, L. (1994). Inhibition Test (72 hours) in Freshwater Unicellular Algae MADAM MECL. Societe d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

(5) Molinier B. (1992). MADQUAT MC 75: Reverse Mutation Assay by the Ames test. Test Report of Elf Atochem S.A. (France).

(6) Molinier B. (1995). MADQUAT MC 75: *In Vitro* Mammalian Cytogenic Test in Cultured Human Lymphocytes. Test Report of Elf Atochem S.A. (France).

(7) Adams, K. (1997). MADAM-MC Mammalian Cell Mutation Assay. Huntington Laboratories, Cambridgeshire, UK.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-15210B1

I U C L I D

Data Set

Existing Chemical	:	Substance ID: 6891-44-7
CAS No.	:	6891-44-7
TSCA Name	:	Ethanaminium, N,N,N-trimethyl-2-[(2-methyl-1-oxo-2-propenyl)oxy]-, methyl sulfate
Structural formula	:	CH3C2H2COOC2H4N.(CH3)3.OSO3CH3
Molecular formula	:	C9H18NO2.CH3O4S

Producer related part

Company	:	Quat HPV Challenge Task Group
Creation date	:	10.11.2003

Substance related part

Company	:	Quat HPV Challenge Task Group
Creation date	:	10.11.2003
Number of pages	:	18
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	Organic.
Physical status	:	Solid.
Purity	:	> 99%.
Remark	:	The commercial product is manufactured and shipped as a solution (75 – 80%) in water.

10.11.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Dimethylaminoethylmethacrylate, dimethyl sulfate
10.11.2003

Choline, methylsulfate, acrylate
10.11.2003

Ethanaminium, *N,N,N*-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, methyl sulfate
10.11.2003

[2-(Acryloyloxy)ethyl]trimethylammonium methyl sulphate
10.11.2003

N,N,N-Trimethyl-2-[(1-oxo-2-propenyl)oxy]ethanaminium methyl sulfate
10.11.2003

N,N,N-Trimethyl-2-(1-oxo-2-propenyloxy)ethanaminium methyl sulfate
10.11.2003

Trimethylammonioethyl acrylate, methylsulfate salt
10.11.2003

(2-Acryloyloxyethyl)-N,N,N-trimethylammonium methosulfate
10.11.2003

MADAMDMS
10.11.2003

DMAEMDMS
10.11.2003

Flocryl MADAMQUAT DMS
10.11.2003

1.3 IMPURITIES

Dimethylaminoethylmethacrylate (<0.1%).
10.11.2003

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

Sensitizing. Irritating to eyes.
10.11.2003

1.6.2 CLASSIFICATION

Not Regulated
10.11.2003

1.6.3 PACKAGING

1.7 USE PATTERN

Type	:	Industrial
Category	:	Chemical industry; used in synthesis of water soluble polymers, flocculants, retention aids.
Remark	:	Commercial product is manufactured and shipped as a solution in water (75–80%).

10.11.2003

1.7.1 DETAILED USE PATTERN

Used in closed system to manufacture polymers. Polymers are water-soluble and cationic and are either copolymers with acrylamide and other monomers or homopolymers.
10.11.2003

1.7.2 METHODS OF MANUFACTURE

Manufactured by reaction of dimethyl sulfate with dimethylaminoethylmethacrylate.
10.11.2003

1.8 REGULATORY MEASURES

None
10.11.2003

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

None.
10.11.2003

1.8.2 ACCEPTABLE RESIDUES LEVELS

Dimethylaminoethylmethacrylate (MADAM) at less than 0.1%.
10.11.2003

1.8.3 WATER POLLUTION

Not applicable.
10.11.2003

1.8.4 MAJOR ACCIDENT HAZARDS

Not applicable.
10.11.2003

1.8.5 AIR POLLUTION

Not applicable.
10.11.2003

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

Listed on all major chemical inventories (TSCA, EINECS, ECL, AICS, etc.).
10.11.2003

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

Not applicable.
10.11.2003

1.9.2 COMPONENTS

Pure substance (in aqueous solution).
10.11.2003

1.10 SOURCE OF EXPOSURE

None.
10.11.2003

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

2.2 BOILING POINT

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

2.5 PARTITION COEFFICIENT

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : Static.
Species : *Brachydanio rerio* (Zebra fish) (Fish, fresh water).
Reference Calmels, R. (1994a).
Exposure period : 96 hours
Unit : mg/l
LC0 : > 100
LC50 : Not observed.
LC50 : Not observed.
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 203, 1984: "Fish, Acute Toxicity Test".
Year : 1994
GLP : No.
Test substance : MADAME DMS
Test procedure : Groups of 10 fresh water Zebra fish (*Brachydanio rerio*) were exposed in a reconstituted medium at 23° C for 96 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Fish mortality was measured after 24, 48 and 96 hours.
Results :

	Mortality		
Test Concentration (mg/L)	24 hours	48 hours	96 hours
0	0	0	0
1	0	0	0
10	0	0	0
100	0	0	0

Since the LC0 at 24, 48 and 96 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : MADAM DMS (80% in solution in water)
Conclusion : MADAMDMS (80% solution in water) is not toxic to freshwater fish at a concentration of 100 mg/l.
Reliability : (1) valid without restriction
Guideline study

10.11.2003 (1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : Static.
Reference Calmels, R. (1994b).
Species : *Daphnia magna* (Crustacean, fresh water)
Exposure period : 48 hours.
Unit : mg/l
EC0 (immobilization) : > 100
EC50 (immobilization) : Not observed.
EC100 (immobilization) : Not observed.
Analytical monitoring : No.

Method : OECD Guidelines for the Testing of Chemicals, No. 202, April 1984: "*Daphnia* sp., Acute Immobilization Test".
Year : 1994
GLP : No.
Test substance : MADAME DMS
Test procedure : Groups of 10 fresh water daphnia (*Daphnia magna*) were exposed in a reconstituted medium at 23° C for 48 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Immobilized daphnia were counted after 24 and 48 hours.
Results :

		Immobilization		
Concentration (mg/L)	No. of daphnia	No. after 24 hours	No. after 48 hours	% after 24 hours
0	20	0	0	0
1	20	0	0	0
10	20	0	0	0
100	20	0	0	0

Since the EC0 at 24 and 48 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : MADAMDMS (80% in solution in water)
Conclusion : MADAMDMS (80% solution in water) has no effect on the swimming behavior of daphnia at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

10.11.2003 (2)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Type : Static.
Reference Licata-Messana, L. (1994).
Species : *Scenedesmus subspicatus* (Algae, unicellular, fresh water)
Exposure period : 72 hours
Unit : mg/l
EC_A50 (I) : $10<EC_A<100$
$EC_\mu50$ (I) : >100
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 201, June 1984: "Alga, Growth Inhibition Test".
Year : 1994
GLP : No.
Test substance : MADAME DMS
Test procedure : Blue-green algae (*Scenedesmus subspicatus*) were exposed in a reconstituted medium at 23° C for 72 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Algal concentrations were measured after 24, 48 and 72 hours.

Results :

	Algal Concentration				
Concentration (mg/L)	Start	24 hours	48 hours	72 hours	% growth inhibition
0	10,000	103,472	725,000	2,867,361	0
1	10,000	93,055	708,333	2,586,111	7
10	10,000	84,722	513,889	2,375,000	21
100	10,000	69,445	194,444	1,294,444	60

The test was terminated after the range-finding phase.

Test substance : MADAMDMS (80% in solution in water)
Conclusion : MADAMDMS (80% solution in water) moderately inhibits the growth of blue-green algae.
Reliability : (1) valid without restriction
Guideline study

10.11.2003 (3)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2 CORROSIVENESS AND IRRITATION

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 OTHER RELEVANT INFORMATION

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

Avoid all contact with the product by ingestion, inhalation or contact with the skin, eyes and clothing. Do not breathe vapors or spray mist. Wash hands and face before breaks and immediately after handling the product.
Store in contact with air. Do not exceed storage temperature of 30°C. Protect from light.
11.11.2003

8.2 FIRE GUIDANCE

This product does not burn in aqueous solution. No special precautions required. In case of fire, wear a self contained breathing apparatus. Keep containers cool during fire with water spray.
11.11.2003

8.3 EMERGENCY MEASURES

If product is inhaled, move to fresh air.
In case of skin contact, rinse and wash contaminated clothing before re-use. Wash contaminated area immediately for at least 15 minutes. In case of persistent skin irritation, consult a physician.
In case of eye contact, rinse immediately with plenty of water for at least 15 minutes. Keep eye wide open while rinsing and lift upper and lower ids to ensure complete removal of chemical. In case of persistent eye irritation, consult a physician.
If swallowed, do not induce vomiting. Rinse mouth (never give anything by mouth to an unconscious person). Call a physician immediately.
11.11.2003

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

Not applicable.
11.11.2003

8.5 WASTE MANAGEMENT

Can be land filled or incinerated when in compliance with local regulations.
11.11.2003

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Calmels, R. (1994a). Test to Evaluate Acute Toxicity (96hours) in Freshwater Fish (*Brachydanio rerio)* Using a static Method MADAME DMS. Societe d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

(2) Calmels, R. (1994b). Test to Evaluate Acute Toxicity (48hours) in Daphnia MADAME DMS. Societe d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

(3) Licata-Messana, L. (1994). Inhibition Test (72 hours) in Freshwater Unicellular Algae MADAME DMS. Societe d'Ecotoxcicologie et de Physico-Chimie (SEPC), Sarcey, France.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT